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Verein zur Förderung der Internationalen Winterschulen in Kirchberg Austria

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Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 26th International Winterschool on:
Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of twenty-five 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
Matthias Staiger, Amelie Biermann	accommodation
Reinhard Meinke	sponsoring
Nils Rosenkranz	registration, finances
Nils Scheuschner	video transfer and recording, internet
Harald Scheel, Emanuele Poliani	receipts, technical assistance
Dirk Heinrich, Andrei Schliwa	technical assistance
Asmus Vierck	website, e-payment
Jan Laudenbach	abstract booklet
Anja Sandersfeld	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, Andreas, Hans, Stephanie, and Siegmars

Chairpersons

C. Thomsen (Berlin)
A. Hirsch (Erlangen)
H. Kuzmany (Vienna)
S. Reich (Berlin)
S. Roth (Seoul)

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F. Mauri (FR)	

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 nanoribbons • Carbon nanotube optics and electronics • Graphene and Carbon nanotube growth and selection • Single-molecule experiments • Applications of molecular nanostructures • Theory of molecular nanostructures • Biomolecule physics and applications • Nanostructure spintronics

INFORMATION FOR PARTICIPANTS

Time and location

The IWEPNM 2012 starts on Saturday, 3 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 10 March, breakfast. There will be a reception party on 3 March, after dinner, and a farewell party including dinner on Friday, 9 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 2012, Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

Tel: ++43 5357 2741, Fax: ++43 5357 2741 200

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

All questions concerning the the IWEPNM 2011 should be directed to:

Prof. Dr. Christian Thomsen,

Institut für Festkörperphysik, Technische Universität Berlin

Hardenbergstr. 36, 10623 Berlin, Germany

Tel: +49-(0)30-31423187, Fax: +49-(0)30-31427705

email: iwepnm-info@physik.tu-berlin.de, Web: <http://www.iwepnm.org>

Participation

Participation at the IWEPNM 2012 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.: +43 664 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 in the Kirchberg/Kitzbühel area, 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.

Proceedings

The contributions to the IWEPM 2012 will be published by Wiley in *physica status solidi*. The expected date for the appearance of the proceedings is October 2012. **Contributions can only be published if they arrive before the 30 April.** The manuscripts will be reviewed within the following weeks. Acceptance of a contribution for presentation at the Winterschool does not automatically include acceptance for publication in the proceedings.

Manuscript preparation

General author instructions with links to the template, style, packages valid for pss (a), (b), and (c) are available at [http://onlinelibrary.wiley.com/journal/10.1002/\(ISSN\)1610-1642a/homepage/2133_authors.S1M.html](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1610-1642a/homepage/2133_authors.S1M.html). Please use either the Word or the LaTeX template, especially for publication in pss (c), since the articles will be produced from the publication-ready manuscript files. In addition, it is the easiest and most accurate way to check the page limits.

Please do not modify any pre-settings in the manuscript templates/style file such as font sizes, margins, and other formats, to avoid an incorrect layout of the publication. Manuscripts with wrong template use may be returned to the authors by the guest editors or the pss editorial office.

Manuscript submission

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If you already have an ID and a password for this system, use them to log in. If not, register by clicking on the respective link. (right side - New User?) Please note that your login information is CASE SENSITIVE. Should you not remember your access data, use the "password help" section on the website. Once you are logged in, the Main Menu will be displayed. To submit your contribution, please click on Author Center.

File names

Please use only Western letters for the file name, and only lower-case letters for the format extension. Please use clear, self-explaining file names, e.g. smith_version2.doc. Please note that after submitting a manuscript, you can no longer modify it.

IWEPNM 2012
CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 4.03.	morning	Loiseau
	morning, after coffee break	Obraztsova
	evening	Kataura
Monday, 5.03.	morning	Kürti
	morning, after coffee break	Schliwa
	evening	Jarillo-Herrero
Tuesday, 6.03.	morning	Kuzmany
	morning, after coffee break	Jorio
	evening	Dinse
Wednesday, 7.03.	morning	Hirsch
	morning, after coffee break	Setaro
	evening	Stampfer
Thursday, 8.03.	morning	Skakalova
	morning, after coffee break	Mauri
	evening	Carroll
Friday, 9.03.	morning	Forro
	morning, after coffee break	Bockrath
	evening	Roth

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

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

Chairpersons please remember: **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 4	Monday March 5	Tuesday March 6	Wednesday March 7	Thursday March 8	Friday March 9
Topics	synthesis and selection of CNT and graphene	graphene and CNT transport	carbon nanotube spectroscopy	chemistry of CNT / graphene; magnetotransport	graphene transport; CNT/graphene applications	non carbon materials; NEMS, doping of graphene
8:30	Growth of high density carbon nanotube forests ROBERTSON	Quantum Transport and Optoelectronics in Graphene Devices JARILLO-HERRERO	Probing Interactions in Single- and Few-Layer Graphene by Optical Spectroscopy HEINZ	Functional groups on nanocarbons SCHLÖGL	Graphene / Boron Nitride Heterostructures GORBACHEV	Single layer MoS ₂ : devices, electronics and mechanics KIS
9:00			Raman characterization of nanocarbons CANCADO		Phonon-mediated superconductivity in graphene by lithium deposition CALANDRA	Collective phenomena in real time and low temperature in low-dimensional transition metal chalcogenides MIHAILOVIC
9:30	Single-Step Structure Sorting of Single-Wall Carbon Nanotubes using Multicolumn Gel Chromatography KATAURA	Quantum transport in suspended bilayer and trilayer graphene LAU	Intrinsic optical properties of free-standing carbon nanotubes and graphene monolayers BERCIAUD	Tuning the electronic structure of low dimensional nanocarbons by means of charge transfer GULDI	Electronic properties of free-standing graphene at low energies ELIAS	How the crystallographic symmetry influences the electronic properties of quantum dots SCHLIWA
10:00	Coffee break					
10:30	Noncovalent Functionalization of Carbon Nanotubes by Designed Surfactants BACKES	Pulse gating on graphene quantum dots STAMPFER	Dominant phonon wavevectors and strain-induced splitting of the 2D Raman mode of graphene NARULA	Reductive Exfoliation of Graphite and Covalent Functionalization of Graphene ENGLERT	Epitaxial graphene nanoribbons BERGER	Electromechanical resonators made from nanotubes and graphene BACHTOLD
11:00	Synthesis of carbon nanostructures from computer simulation BICHARA	Quantum Transport in Disordered Graphene ROCHE	Theory of Raman spectroscopy of graphene on different substrates WIRTZ	Advances in understanding Chemistry of Graphene and CNTs: Fundamentals and Applications STRANO	Light-matter interaction in a microcavity-controlled graphene transistor ENGEL	Ultrastrong Adhesion and other Graphene Mechanical Wonders BUNCH
11:30	Preparation and applications of single- and multiple-wall arrays KANELLOPOULOS	Level structure and tunnel couplings of carbon nanotube quantum dots GROVE-RASMUSSEN	Double-resonant Raman modes in few-layer graphene MAULTZSCH	From organic monolayers to carbon nanomembranes and graphene with tunable structural, chemical and electrical properties TURCHANIN	Electronic properties of organic materials: small molecule field-effect transistors and graphene WEITZ	Strain, wrinkles and other aspects of the thinnest crystalline membrane PEREIRA

12:00-17:00	Mini workshops					
17:00 - 18:30	Dinner					
18:30	Repeated CVD Growth of Single Crystal Graphene with Millimeter Size and Its Nondestructive Transfer CHENG	Photoinduced currents in graphene and carbon nanotubes IVCHENKO	ESR from fully metal - semiconductor separated SWCNTs CHERNOV	Spin transport in graphene GÜNTERTROTH	Catalytically Grown Carbon Nanotubes ENDO	17:00 Electron-Phonon Interactions in quasi-free-standing Graphene HABERER-GEHRMANN
19:00	Complementary in-situ probing of graphene CVD HOFMANN	Gate tuning of electronic states in nanosheets IWASA	Ultrafast confocal microscopy and CT dynamics LANZANI	Magnetism in graphene induced by point defects GRIGORIEVA	Single wall carbon nanotube based electronic junction control devices RINZLER	17:30 Superstructuring of graphene: charge-transport in superlattices KRSTIC
19:30	Graphene Magnetism and Spintronics HARUYAMA	Superconductivity in Bundles of Double-Wall Carbon Nanotubes SHENG	Electronic transport properties of functionalized metallicity sorted single walled carbon nanotubes PICHLER	Unconventional Sequence of Fractional Quantum Hall States in Suspended Graphene FELDMAN	Probing Charge Transfer and Photothermoelectric Responses from SWNT Devices MARTEL	18:00 IWEPM12 - Conference summary JORIO
20:00	The physics and chemistry of sp-2 bonded carbon explored by high-resolution electron microscopy MEYER	Poster I Monday	Poster II Tuesday	Spin and Magnetism in Graphene KAWAKAMI	Poster III Thursday	Bauernbuffet Farewell
20:30						
Topics	synthesis and selection of CNT and graphene	graphene and CNT transport	carbon nanotube spectroscopy	chemistry of CNT / graphene; magnetotransport	graphene transport; CNT/graphene applications	non carbon materials; NEMS, doping of graphene
	Sunday March 4	Monday March 5	Tuesday March 6	Wednesday March 7	Thursday March 8	Friday March 9

PROGRAM

AND

ABSTRACTS



- Size-based separation of soluble carbon nanotubes
- Hydrophilic group coating silica packing material
- Three types of pore sizes (300 Å, 1000 Å, 2000 Å)
- High durability

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Synthesis and selection of CNT and graphene

Sunday, March 4th

- 08:30 – 09:30 **J. Robertson, Cambridge**
Growth of high density carbon nanotube forests
- 09:30 – 10:00 **H. Kataura, Tsukuba**
Single-Step Structure Sorting of Single-Wall Carbon Nanotubes using Multicolumn Gel Chromatography
- 10:00 – 10:30 **Coffee break**
- 10:30 – 11:00 **C. Backes, Erlangen**
Noncovalent Functionalization of Carbon Nanotubes by Designed Surfactants
- 11:00 – 11:30 **C. Bichara, Marseille**
Synthesis of carbon nanostructures from computer simulation
- 11:30 – 12:00 **N. Kanellopoulos, Athens**
Preparation and applications of single- and -multiple wall arrays
- 12:00 – 17:00 **Mini-Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **H. Cheng, Shenyang**
Repeated CVD Growth of Single Crystal Graphene with Millimeter Size and Its Nondestructive Transfer
- 19:00 – 19:30 **S. Hofmann, Cambridge**
Complementary in-situ probing of graphene CVD
- 19:30 – 20:00 **J. Haruyama, Kanagawa**
Graphene Magnetism and Spintronics
- 20:00 – 20:30 **J. Meyer, Wien**
The physics and chemistry of sp² bonded carbon explored by high-resolution electron microscopy

Sunday, March 4th

Synthesis and selection of CNT and graphene

08:30**Growth of high density carbon nanotube forests**John Robertson¹, G Zhong¹, S Esconjauregui¹, C Zhang¹, M Fouquet¹, A H Warner², S Hofmann¹¹Engineering Dept, Cambridge University, Cambridge²Oxford University

The talk will review progress on growth of dense vertically aligned carbon nanotube forests by catalytic chemical vapor deposition (CVD), how to maximise forest height and what ultimately limits catalyst lifetime. There is also debate about whether preferential nucleation of caps or different growth rates leads to a preference for armchair tubes, and what can lead to chirality selection. In-situ TEM and XPS shows the state of the catalyst during growth. Nevertheless, standard forests have only 0.05 of the maximum possible density. Some applications such as CNT interconnects or heat spreaders need much higher area density. Higher density is possible by better catalyst design. The CNT area density closely follows the area density of the original catalyst nanoparticles, as formed by thermal annealing of the initial catalyst film. In addition, densities can be maximised for small CNT diameters, as density varies as $1/D^2$. We show how sequential deposition and annealing of catalyst, or careful treatment of the support layer can increase nucleation density. Also, various strategies to immobilise the catalyst by plasma treatment can increase densities towards the theoretical limit.

09:30**Single-Step Structure Sorting of Single-Wall Carbon Nanotubes using Multicolumn Gel Chromatography**Hiromichi Kataura^{1,2}, Huaping Liu^{1,2}, Maki Shimizu^{1,2}, Yasuhiro Ito^{1,2}, Shunjiro Fujii^{1,2}, Takeshi Tanaka¹¹Nanosystem Research Institute, AIST, Tsukuba, Japan²CREST, JST, Kawaguchi, Japan

Mixed production of metallic and semiconducting single-wall carbon nanotubes (SWCNTs) with a variety of diameters is one of the most serious problems for their electronic device applications. To solve this problem, we have developed multicolumn gel chromatography method for the precise structure sorting of semiconducting (S-) SWCNTs using commercially available Sephacryl gel [1]. Applying this method twice to HiPco SWCNTs, we could sort out 13 kinds of S-SWCNTs by the difference in the local C-C bond curvature. However, this two-step separation method is not effective to be applied to the large scale separation. For the further improvements, we have analyzed separation mechanism and then found that it is possible to control the interaction between S-SWCNTs and the Sephacryl gel by changing surfactant concentration and the system temperature. Finally, we succeeded in simplifying the separation procedure and 7 kinds of single chirality S-SWCNTs were obtained by the single step multicolumn method. In this presentation, we will show the detailed procedure of the multicolumn method and the future perspective.

References [1] H. Liu et al. Nat. Commun., 2 (2011) 309.

10:30**Noncovalent Functionalization of Carbon Nanotubes by Designed Surfactants**Claudia Backes¹, Andreas Hirsch²¹Cluster of Excellence Engineering of Advanced Materials, University Erlangen-Nuremberg, Erlangen²Chair of Organic Chemistry, University Erlangen-Nuremberg, Erlangen

Single-walled carbon nanotubes (SWCNTs) rank among the most fascinating materials of the 21st century. However, SWCNT-based technology has commenced slowly due to two major hurdles that need to be overcome: their poor solubility in common solvents and the polydispersity of the as-produced material. Up to now, despite the extraordinary progresses in the development of SWCNT sorting techniques, the efficiency of the separation has been restricted by the limited exfoliation power of commercially available detergents. This is exactly the point, where this contribution hooks in, in order to pave the way to improved sorting.

Fundamental insights in noncovalent SWCNT functionalization by π -surfactants are presented with the focus on establishing structure-property relationships of adsorbates and SWCNTs in aqueous solution to understand the dispersion behavior. By the aid of designed surfactants based on perylene bisimide derivatives, SWCNT exfoliation is greatly enhanced and concepts for sorting are developed.

C. Backes, F. Hauke, A. Hirsch, *Adv. Mater.* 2011, 23, 2588.

C. Backes, *Springer Theses*, Springer Berlin Heidelberg, 2012, ISBN 978-3-642-27581-4.

11:00**Synthesis of carbon nanostructures from computer simulation**Christophe Bichara¹¹CINaM, CNRS and Aix Marseille University, Marseille

The outstanding electronic, optical and transport properties of carbon nanotubes and graphene critically depend on the quality of their atomic scale structure. However, nanostructures that are actually produced are far from being ideal and the large scale synthesis of nanostructures with designed properties is not yet achieved, mainly because of our limited understanding of the nucleation and growth mechanisms at the atomic scale. Atomistic computer simulation is ideally suited for investigations at this scale.

Here, we use a carefully assessed tight binding model for nickel and carbon coupled to grand canonical Monte Carlo simulations, to calculate carbon adsorption isotherms on Ni slabs and nanoparticles (NP). We can thereby study the chemical and physical state of the metal catalyst under growth conditions for SWNTs and graphene. Combining TEM and atomistic computer simulation we study the relation between the tube diameter and the NP from which it grows. We then study the growth of tube butts with different chiralities under different chemical potential and temperature conditions to try and preserve the initial tube structure.

Synthesis and selection of CNT and graphene

Sunday, March 4th

11:30

Preparation and applications of single- and -multiple wall arrays

Nick Kanellopoulos¹

¹Institute of Physical Chemistry, NCSR Demokritos, Athens

18:30**Repeated CVD Growth of Single Crystal Graphene with Millimeter Size and Its Nondestructive Transfer**Hui-Ming Cheng¹, Libo Gao¹, Wencai Ren¹, Li Jin², Zhenxing Wang³, Qiang Fu², Zhiyong Zhang³, Xinhe Bao², Lian-Mao Peng³¹Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China²State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China³Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China.

Large-size grains are important for the applications of graphene since grain boundaries are believed to markedly degrade its quality and properties. However, graphene films prepared so far are usually stitched together from nanometer to micrometer-size grains. Moreover, the current transfer methods of graphene are mainly based on substrate etching, which leads to inevitable damage of metal substrates and worsens environments. We will report the growth of graphene films with millimeter-size single crystal hexagonal grains on polycrystalline Pt foils by ambient pressure chemical vapour deposition (CVD). Furthermore, a bubbling method has been developed to transfer these graphene films, which is nondestructive to the Pt foils. The Pt foils can be repeatedly used for graphene growth with no limit. The graphene film has high crystallinity, high electrical conductivity, and the smallest mean amplitude of wrinkles 0.8 nm ever observed. The CVD growth of high-quality single-crystal graphene with large-size grains on repeatably usable metal substrates enables numerous applications, in particular for electronics and optoelectronics at a low cost.

19:00**Complementary in-situ probing of graphene CVD**Stephan Hofmann¹, R.S. Weatherup¹, B.C. Bayer¹, P.R. Kidambi¹, R. Blume², C. Baehtz³, R. Schlögl⁴¹University of Cambridge, Cambridge²Helmholtz-Zentrum Berlin für Materialien und Energie, Germany³Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, Germany⁴Fritz Haber Institute, Germany

Chemical vapor deposition (CVD) is the most promising technique for scalable and economical mono- and few-layer graphene (M-/FLG) growth, a key requirement for future device applications. The current understanding of the M-/FLG growth processes, however, is very limited and key questions remain open, such as what M-/FLG quality can be achieved with CVD, in particular, if for cost effectiveness sacrificial poly-crystalline metal films/foils and less stringent vacuum/CVD process conditions are used. We study M-/FLG CVD by complementary in situ probing under realistic process conditions with the aim of revealing the dominant growth mechanisms. Here we focus on high-pressure XPS and in-situ XRD of model polycrystalline Ni catalyst films [1,2] and show that M-/FLG growth occurs during isothermal hydrocarbon exposure and is not limited to precipitation upon cooling. We show that alloying Ni with Au allows low temperature (<450C) CVD of predominantly MLG films (>74%) with an average D/G ratio of ~ 0.24 and domain sizes in excess of $220\mu m^2$. Au alloying drastically lowers the graphene nucleation density, allowing more uniform and controlled growth at CMOS compatible temperatures.

[1] Weatherup et al. Nano Lett. 11, 4154, 2011

[2] Weatherup et al. ChemPhysChem, 2012

19:30**Graphene Magnetism and Spintronics**Junji Haruyama¹¹Aoyama Gakuin University, Kanagawa

Although a variety of phenomena has been experimentally reported in graphenes, mostly none have experimentally reported edge-related phenomena, because lithographic fabrication of edges introduces defects. Basically, there are two kinds of atomic structures in graphene edges; arm chair and zigzag. Theoretically, arm chair edge gives band gap opening, while zigzag edge yields a flat energy band, resulting in electron localization and polarization. Here, we have developed two non-lithographic methods; (1) graphene nanoribbons (GNRs) derived from unzipping of carbon nanotubes with annealing and (2) graphene nanopore arrays (GNPAs) fabricated using porous alumina template. I talk that the low-defect GNRs with arm chair edges can have band gaps 7-times greater than large-defect GNRs [1] and that the GNPAs with zigzag edges exhibit ferromagnetism [2] and anomalous magnetoresistance oscillations [3]. The zigzag-GNPAs must open a door to carbon-based spin physics and spintronics. [1] T.Shimizu, J.Haruyama et al., Nature Nanotech.6, 45 (2011) [2] K. Tada, J. Haruyama et al., PRL 107, 217203 (2011) [3] T. Shimizu, J. Haruyama et al., APL 100, 023104 (2012)

20:00**The physics and chemistry of sp-2 bonded carbon explored by high-resolution electron microscopy**

Jannik C Meyer^{1,2}, Jani Kotakoski^{1,3}, Simon Kurasch², Franz Eder¹, Viera Skákalová¹, Benedikt Westenfelder⁴, Johannes Biskupek², Ferdinand Scholz⁴, Carl E. Krill III⁵, Arkady V. Krasheninnikov^{3,6}, Ute Kaiser²

¹Department of Physics, University of Vienna, Wien, Austria

²Central facility for electron microscopy, University of Ulm, Ulm, Germany

³Department of Physics, University of Helsinki, Helsinki, Finland

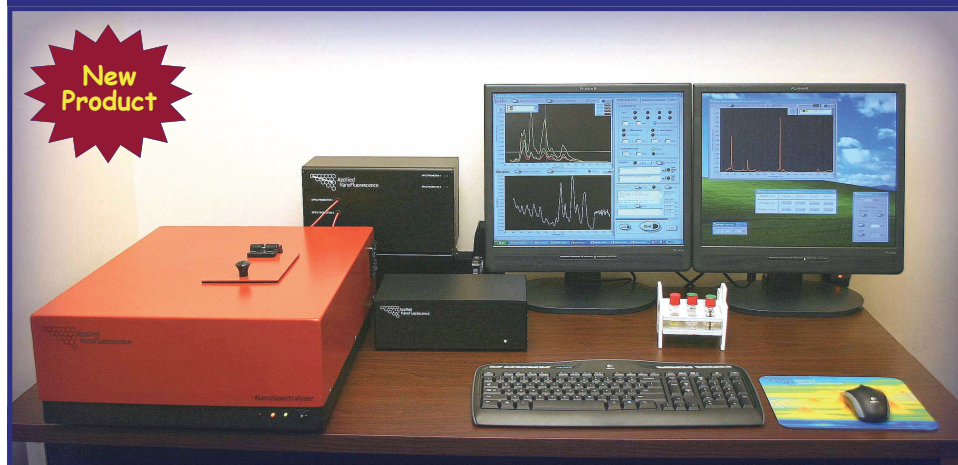
⁴Institute of Optoelectronics, University of Ulm, Ulm, Germany

⁵Institute of Micro and Nanomaterials, University of Ulm, Ulm, Germany

⁶Department of Applied Physics, Aalto University, Aalto, Finland

The study of nano-carbons and other low-atomic number materials remains a particular challenge for high resolution electron microscopy owing to their intrinsically low contrast and high susceptibility to radiation damage. We analyzed the mechanisms behind beam-driven structural changes and demonstrate how a controlled modification, beyond the ejection of atoms, can be achieved. An electron beam can be used to selectively suppress and enhance bond rotations and atom removal in graphene, which allows to turn graphene into a two-dimensional coherent amorphous membrane composed of sp²-hybridized carbon atoms. In addition, substitutional doping of graphene can be obtained not only via a modified synthesis but also by electron irradiation effects. Here, the direct visualization of nitrogen dopants in graphene was demonstrated along with an analysis of charge redistribution around the defect. The graphene substrate may further serve as an extreme thermal test platform, which then provides a means to study physisorbed carbon species under the influence of high temperatures and electron irradiation.

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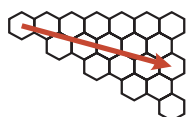
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Applications: SWCNTs, MWCNTs,
graphene, quantum dots, singlet oxygen

Capability	NS1	NS2	NS3
Near-IR emission	✓	✓	✓
Near-IR absorption	✓	✓	✓
Visible absorption	O	✓	✓
Raman (1 laser)		✓	O
Raman (2 lasers)			O
Visible emission			O
Extended NIR em/abs			O
UV absorption			O
Vertical sample scanning		O	O

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Graphene and CNT transport

Monday, March 5th

- 08:30 – 09:30 **P. Jarillo-Herrero, Cambridge**
Quantum Transport and Optoelectronics in Graphene Devices
- 09:30 – 10:00 **C. Lau, Riverside**
Quantum transport in suspended bilayer and trilayer graphene
- 10:00 – 10:30 **Coffee break**
- 10:30 – 11:00 **C. Stampfer, Aachen**
Pulse gating on graphene quantum dots
- 11:00 – 11:30 **S. Roche, Barcelona**
Quantum Transport in Disordered Graphene
- 11:30 – 12:00 **K. Grove-Rasmussen, Copenhagen**
Level structure and tunnel couplings of carbon nanotube quantum dots
- 12:00 – 17:00 **Mini-Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **E. Ivchenko, Saint-Petersburg**
Photoinduced currents in graphene and carbon nanotubes
- 19:00 – 19:30 **Y. Iwasa, Tokyo**
Gate tuning of electronic states in nanosheets
- 19:30 – 20:00 **P. Sheng, Hong Kong**
Superconductivity in Bundles of Double-Wall Carbon Nanotubes
- 20:00 **Poster I**

Monday, March 5th

Graphene and CNT transport

08:30**Quantum Transport and Optoelectronics in Graphene Devices**Pablo Jarillo-Herrero¹¹MIT, Cambridge

Over the past few years, the physics of low dimensional electronic systems has been revolutionized by the discovery of materials with very unusual electronic structures. Among these, graphene has taken center stage due to its relativistic-like electron dynamics and potential applications in nanotechnology. Moreover, the recent discovery that hexagonal boron nitride (hBN) is a nearly-ideal substrate for high mobility graphene devices has enabled a new generation of quantum transport experiments in graphene. In this talk I will review our recent experiments on few layer graphene devices on hBN in the quantum Hall regime, including trilayer and twisted bilayer graphene. In addition I'll review our optoelectronic experiments on graphene pn junctions, where we observe a hot-carrier mediated photothermoelectric intrinsic graphene optical response.

09:30

Quantum transport in suspended bilayer and trilayer graphene

Chun Ning Jeanie Lau¹

¹University of California, Riverside, Riverside

Graphene, a two - dimensional single atomic layer of carbon, has recently emerged as a promising candidate for electronic materials, as well as a new model system for condensed matter physics. In this talk I will present our results on transport measurements in bilayer and trilayer suspended graphene devices. In these ultra-high mobility devices, we demonstrate intrinsic gapped insulating state at the charge neutrality point, evidence for quantum phase transitions, and stacking-order dependent transport. Our work contributes towards understanding the rich interaction-driven physics in few layer graphene.

10:30**Pulse gating on graphene quantum dots**Christoph Stampfer^{1,2}, Christian Volk^{1,2}, Christoph Neumann¹, Stephan Engels^{1,2}, Jan Dauber^{1,2}, Bernat Terres^{1,2}, Stefan Trellenkamp², Sebastian Kazarski¹¹JARA-FIT and II. Institute of Physics B, RWTH Aachen University, Aachen²Peter Grünberg Institute, Forschungszentrum Jülich, Jülich

Graphene quantum dots (QDs) have received increasing attention over the last years, mainly due to their promise for implementing spin qubits. Compared to well-established GaAs-based QDs, their smaller hyperfine and spin-orbit coupling promises more favorable spin coherence times. However, while the preparation, manipulation, and read-out of single spins have been demonstrated in GaAs, research on graphene QDs is still at an early stage. Although Coulomb blockade phenomena and excited state spectroscopy is now well established, experimental signatures allowing the identification of relaxation times have been hard to trace. Here we report on the current status of pulse gating experiments on graphene quantum devices and in particular we will present measurements of the charge relaxation rates in single-layer graphene QDs. The investigated devices consist of an island with a diameter of 120 nm, 4 lateral graphene gates and 2 charge detectors. From so-called diamond measurements we extract a charging energy of 11 meV and excited state level spacings on the order of 2-4 meV. Low-bias pulse gate measurements allow finally to extract relaxation rates on the order of 50 ns.

11:00**Quantum Transport in Disordered Graphene**Stephan Roche¹¹Catalan Institute of Nanotechnology, Barcelona

This talk will focus on the presentation of transport properties in disordered graphene-based-materials, driven by chemical functionalization and structural defects. By using state-of-the-art multiscale simulations (combining first-principles with tight-binding schemes), we present several electronic transport features in complex forms of chemically modified and disordered graphene based materials. Conditions to observe crossovers from weak localization to weak antilocalization regimes will be first discussed, followed by a description of localization phenomena driven by structural defects and oxygen ad-atoms. Finally, the effect of atomic hydrogen driving intrinsic magnetic ordering will be presented. The existence of a long range ferromagnetic state in weakly hydrogenated graphene will be related to a highly robust metallic state down to cryogenic temperatures, in contrast to the localization regime obtained in absence of ferromagnetic order. The possibility to observe measurable magnetoresistance signals due to magnetism in graphene will be finally addressed.

11:30**Level structure and tunnel couplings of carbon nanotube quantum dots**Kasper Grove-Rasmussen¹¹Niels Bohr Institute & Nano-Science Center, University of Copenhagen, Denmark

We present low temperature transport measurements of a carbon nanotube quantum dot in parallel and perpendicular magnetic fields allowing us to study the quantum levels of the system. The observed energy spectrum consisting of near four-fold degenerate shells (two split doublets) is shown to be well understood within a simple one-shell model including disorder-induced valley mixing and spin-orbit interaction [1]. For certain shells, the two doublets are differently tunnel coupled to the leads, resulting in gate-dependent level renormalization. By comparison to the one-shell model this is shown to be a consequence of valley mixing in the nanotube. Moreover, a parallel magnetic field is shown to reduce this mixing and thus suppress the effects of tunnel renormalization [2].

[1] T. Sand Jespersen, K. Grove-Rasmussen, J. Paaske, K. Muraki, T. Fujisawa, J. Nygård, and K. Flensberg, *Nat. Phys.* 7, 348 (2011).

[2] K. Grove-Rasmussen, S. Grap, J. Paaske, K. Flensberg, S. Andergassen, V. Meden, H. I. Jørgensen, K. Muraki, and T. Fujisawa, submitted (2011).

18:30**Photoinduced currents in graphene and carbon nanotubes**E. L. Ivchenko¹¹Ioffe Physical-Technical Institute, Saint-Petersburg, Russia

In my talk I overview experimental and theoretical studies of photogalvanic effects (PGE) in graphene and carbon nanotubes. The following items are to be discussed.

(i) Photon drag effect, or the dynamic Hall effect, induced in single-layer graphene under oblique incidence of the terahertz and infrared radiation. The second-harmonic generation as complementary to the drag photocurrent. Chiral edge currents in graphene samples generated by illumination of the edges at normal incidence.

(ii) Pure valley currents under the homogeneous normal-incidence photoexcitation of graphene. The intravalley current appears because of the reduced symmetry D_{3h} of the valleys K and K' while the net electric current is forbidden by the overall D_{6h} point-group symmetry.

(iii) Photogalvanic properties of graphene superlattices (SLs) formed by periodic strain. Asymmetric graphene SLs act as quantum ratchets and allow helicity-dependent photocurrents.

(iv) Effects inherent for chiral carbon nanotubes: circular PGE, magneto-induced linear PGE, natural circular dichroism, magneto-chiral dc electric current quadratic in the bias voltage applied to a chiral nanotube.

19:00**Gate tuning of electronic states in nanosheets**Yoshi Iwasa^{1,2}¹QPEC & Department of Applied Physics, University of Tokyo, Japan²RIKEN ASI, Correlated Electron Research Group, Japan

Electric double layer (EDL), self-organized at the interface between solid-liquid interfaces, is an electrochemical concept proposed by Helmholtz 150 year ago. We emphasize that the electric field at EDLs can be as large as 50 MV/cm, which is more than one order of magnitude larger than that realized in all solid devices. This electric field produces two dimensional electron systems (2DES) with extremely high carrier density, which is also more than one order larger than that in solid devices. To probe this 2DES, we fabricated electric double layer transistor (EDLT), which has a device configuration equivalent to the field effect transistors. We applied this technique to a variety of materials to establish a new paradigm of materials science at ultrahigh electric fields. We have so far demonstrated electric field induced superconductivity, ferromagnetism, and gate-tuned multisubband transport in graphene and carbon nanotubes. In this presentation, we discuss on the gate tuning of electronic states in several nanosheets, involving graphene and layered materials fabricated by a Scotch-tape technique, with particular focus on electric field induced superconductivity.

19:30**Superconductivity in Bundles of Double-Wall Carbon Nanotubes**Ping Sheng¹¹Department of Physics, Hong Kong University of Science and Technology, Hong Kong

We present electrical and thermal specific heat measurements that are in support of superconductivity in selective samples of double-wall carbon nanotube bundles. Clear evidence, comprising a resistance drop as a function of temperature, magnetoresistance and differential resistance signatures of the supercurrent, suggest an intrinsic superconducting transition below 6.8 K for one particular sample. Additional electrical data from four other sample devices, out of the 22 sample devices that display superconducting behavior (in a total 200 devices made and tested), are also presented not only to confirm the existence of superconductivity but also to give some indication about the abundance of the superconducting species and their T_c distribution. Raman characterization for one of these selective samples shows the inner tube to be metallic and the outer tube to be semiconducting in character. A broad superconducting anomaly is also observed in the specific heat data of a bulk double-wall carbon nanotube sample, which yields a T_c distribution that correlates well with the distribution obtained from the electrical data.

MON 1**On the ionization of C_{60} fullerene in laser desorption/ionization mass-spectrometry: influence of solvation**

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The fine structure and rate of clusterization in mass-spectra (laser desorption/ ionization, LDI) of C_{60} fullerene precipitated from solutions of various polarity (carbon disulfide, toluene, benzene, N-methyl-2-pyrrolidone) is sensitive to the state of fullerene molecules in the initial solution. It is supposed that the residual solvent molecules as components of precipitates affect the ionization, as well as the accompanying fragmentation and clusterization in the LDI process. The effect is stronger for the solutions with higher polarity. The influence of the appearance, growth and reorganization of fullerene aggregates in initial polar solutions on the mass-spectra is also observed and is in agreement with the results of other complementary methods (extraction, small-angle scattering, NMR). Thus, it is shown that mass spectrometry experiments can be used to get information on the solute-solvent interaction.

MON 2**Covalent functionalization of carbon nanotubes with electro-active groups for bioelectrochemical applications.**

Naoual Allali^{1,2}, Victor Mamane¹, Veronika Urbanova², Mathieu Etienne², Xavier Devaux³, Brigitte Vigolo⁴, Maxime Noël⁵, Alain Walcarius², Alexander V. Soldatov⁵, Yves Fort¹, Edward McRae⁴, Manuel Dossot²

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Carbon nanotubes (CNTs) present a strong potential interest for developing bioelectrochemical devices owing to their electronic properties, their high surface area

and the possibility to graft electro-active chemical groups on their side-walls, which can promote the electron transfer between the target enzyme and the electrode. We present here our strategy for covalently functionalizing CNTs to improve both their water dispersion efficiency and their electro-chemical activity. The facilitating of water dispersion will allow the functionalized CNTs (f-CNTs) to be deposited at the electrode directly from the suspension, with no solvent or other surfactant molecule. We will use these f-CNTs to make an electro-chemical device based on the use of the cofactor NADH (dihydronicotinamide adenine dinucleotide). We report i) the covalent functionalization of CNTs by modified electro-active groups, ii) the complete characterization of f-CNTs by spectroscopic, thermal and microscopic methods, iii) the integration of these f-CNTs within electro-chemical devices and iv) the final electrochemical characterization of the full device.

MON 3

Synthesis and characterization of C₆₀ Peapods and DWCNTs

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Filling the single-walled carbon nanotubes' (SWCNTs) cavity with fullerene molecules or with an inner tube will alter the electronic and mechanical properties of the nanotubes. It is also possible to fine-tune the properties by changing the filler [1]. There is an optimum diameter of the SWCNTs for the interaction between the filler and the tube's wall [2]. Here, we report the preparation of high yield of SWCNTs encapsulating C₆₀ fullerene molecules and also the preparation of double-walled carbon nanotubes (DWCNTs) derived from the C₆₀ peapods. The prepared samples were characterized by aberration-corrected HRTEM, Raman, and infrared spectroscopy. The possibility of the interaction between the fillers (fullerene molecules, tube) and the SWCNT will be discussed.

[1] F. Simon et al., Chem. Phys. Lett. **383**, 362 (2004). [2] A. G. Ryabenko et al., Carbon **45**, 1492 (2007).

MON 4

Strain enhancement by PPy modification of bucky gel actuators

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Bucky gel actuators are attractive because they can operate at low voltage in air with promising frequency and strain performance, which can be significantly improved by a combination of physical and chemical modifications together with appropriate engineering. We showed that it is possible to increase the performance of such actuators by cross-linking carbon nanotubes (CNTs) with an aromatic diamine (PPD). Here we present novel results obtained cross-linking super growth CNTs by a cyclic aliphatic diamine (DCH). Moreover we demonstrate that it is possible to synthesize PPy on the surface of the jellified CNTs by using AuCl_3 as oxidant in ionic liquid medium and this leads to the fabrication of actuators that, compared to pure CNT based ones, display a maximum strain up to five times larger. Another limit of existing technology for bucky gel artificial muscles is their bimorph configuration. We designed a novel three electrode actuator capable of both linear and bending motion. Finally, we propose a way to model actuation performance in terms of purely material-dependent parameters instead of geometry-dependent ones. Our latest results will be discussed.

MON 5

Simple Dip-Coating Process for Synthesis of Highly Pure Small Diameter Single Walled Carbon Nanotubes – Effect of Catalyst Composition on Chirality Distributions

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We report on a simple dip-coating method to prepare catalyst particles (mixture of iron and cobalt) with a controlled diameter distribution on silicon wafer substrates by changing the solution concentration and withdrawal velocity. The size and distribution of the prepared catalyst particles were analyzed by atomic force microscopy. Carbon nanotubes were grown by chemical vapor deposition on the substrates with prepared catalyst particles. By decreasing the catalyst particle size, the growth of carbon nanotubes can be tuned from few walled carbon nanotubes, with homogeneous diameters, to highly pure single-walled carbon nanotubes. Analysis of the Raman radial breathing modes, showed a relatively broad diameter distribution (0.8 nm – 1.4 nm) of single-walled carbon nanotubes with different chiralities. By changing the size and composition of the catalyst particles but maintaining the growth parameters, the chiralities of single-walled carbon nanotubes were reduced to mainly four different types: (12, 1), (12, 0), (8, 5) and (7, 5) of which quantity is 70 % of all nanotubes.

MON 6**Tunnelling through ultrathin boron nitride crystals**

B. D. Belle¹, L. Britnell², R. V. Gorbachev¹, R. Jalil¹, F. Schedin¹, M. I. Katsnelson³, L. Eaves⁴, S. V. Morozov⁵, N. M. R. Peres⁶, A. H. Castro Neto^{6,7}, J. Leist⁸, A. K. Geim^{1,2}, L. A. Ponomarenko², K. S. Novoselov²

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⁸Momentive Performance Materials, OH

Hexagonal boron nitride (h-BN) is a member of the two-dimensional atomic crystal family which has seen a recent spark in interest. Most studies up till now have focused on the use of BN as a substrate for graphene electronics. However, it would be beneficial to investigate the performance of BN as a dielectric down to single layers thickness. Ultrathin dielectrics like this would be extremely useful in various devices for flexible electronics. Electron tunnelling through ultrathin boron nitride crystals, contacted by various metals, has been measured down to the thickness of a single layer. Even at such ultimately small thicknesses, boron nitride is found to behave as a high quality insulator where the tunnelling current follows an exponential dependence on the thickness of the boron nitride. Mapping the local tunnelling current across few layer boron nitride terraces shows little variation in current suggesting a low density of defects. Its high breakdown field strength and homogeneity mean BN can be a good choice of material for ultrathin dielectrics for field-effect transistors, allowing high carrier densities to be achieved.

MON 7**The antibacterial studies of nanocrystalline diamond**

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In this study we investigated the potential antibacterial properties of diamond. We tested the samples of nanocrystalline diamond (NCD) film treated by either oxygen or hydrogen plasma and nano-diamond powder (DP). Silica glass and copper were used for negative and positive control samples, respectively. *Escherichia*

coli and *Bacillus subtilis* were used as representatives of Gram negative and Gram positive bacteria, respectively. The outputs of pilot experiments indicate that the antibacterial effect of NCD is limited to the direct contact of bacteria with its surface. The preliminary results of dehydrogenase activity assay and tests on liquid and solid media imply that the potential antibacterial properties of NCD are probably short time and distance limited due to lack of free diffusion. This observation could be the result of death cell biomass deposition on thin layers which will be further discussed. The influence of DP on cells growing in liquid culture is investigated as an alternative concept to the NCD film. Finally, bacterial adhesion on NCD films will be presented too.

MON 8

Growing Graphene Flakes on Titanium Nitride (TiN) substrate

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For the use of Graphene in electronic application it is important to grow thin, single layer graphene on metallic substrates. Titanium Nitride (TiN) substrates are good alternative because of high electrical conductivity and low diffusion coefficient. In this paper we have tried to prepare Graphene on Sputter deposited TiN films by CVD. Thermal stability of TiN substrates was studied up to growth temperature (600oC) via in – situ measurement with XPS and the Graphene growth was done by CVD. It was found that the TiN films, prepared by Sputter deposition are not stable at 600oC and starts forming cracks at higher temperature and have weak adhesion. There are formation of not only Graphene flakes but also small amount of CNTs, which are very small and randomly distributed. The graphene flakes formed were analysed by SEM, Raman and IPES.

MON 9

Electron-phonon coupling in zinc blende and wurtzite CdSe-CdS heteronano-crystals

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Colloidal CdSe-CdS core-shell nanocrystals are currently of high interest because they offer new applications e.g. in photovoltaics. The possibility to synthesize defined nanocrystals with a precise control over their size enables the use in systems like biological sensors, LEDs, lasers and solar cells. The magnitude of the coupling of excited carriers to phonons in the CdSe contributes to the time scales of different photophysical processes of high significance for those applications. These processes

ses include for example carrier multiplication rates, and relaxation times and are strongly influenced by the states in interface region of core and shell. We employ a combined approach of two spectroscopic techniques, Raman spectroscopy and photoluminescence, finding a systematic decrease of the coupling with increasing shell thickness. For the first time we analyze the coupling in the zinc blende and the wurtzite lattice configuration. We find a larger Huang-Rhys factor in wurtzite than zinc blende CdSe nanocrystals. These results can be used to optimize the synthesis parameters to the specific needs of different optical applications.

MON 10**Functionalization of carbon nanotubes with optical dipole switches**

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We report on the efficient solubilization and individualization of carbon nanotubes using different spiropyran based surfactants. Spiropyran serves as an optically addressable dipole switch and is able to influence the properties of the tubes, such as band structure and ballistic transport, depending amongst others on the switching state. We investigate the tube/switch interaction by varying the compound morphology. We present investigations on the distance dependency of tube/switch interaction using two pyrene-spiropyran dyads with spacers of different lengths, resulting in different tube/switch separations. In the case of the shorter spacer, the nanotubes' luminescence as well as the merocyanine absorption band were red-shifted and, furthermore, the rate of the merocyanine to spiropyran thermal back isomerization was decreased.

MON 11**DNA Assembly of Carbon Nanotube Arrays, and Suspended Graphene Break Junctions**

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Parallel arrays of carbon nanotubes are synthesized by using appropriate DNA linker complexes acting as spacers and tethers. Self-assembly occurs when nanotubes diffuse on surfaces such as mica to form into parallel arrays. Varying the length of the spacer sequence can tune the inter-nanotube spacing from a few nm to 20 nm with nm scale precision. Chemically modified DNA produces functional templates with a pre-determined spacing to the carbon nanotubes. Using this we bind streptavidin to biotin linkers placed a few nm away from the nanotubes. Moreover, experiments on narrow gaps formed in suspended single to few layer graphene devices using a pulsed electrical breakdown technique will also be discussed.

The device conductance can be programmed to ON and OFF states by applying voltage pulses. Electron microscope imaging shows that the graphene sheets typically remain suspended and that the device conductance tends to zero when the observed gap is large. The switching rate is strongly temperature dependent, which rules out a purely electromechanical switching mechanism. This demonstrates switching in an all-carbon device, suitable for integration with graphene electronics.

MON 12

Luminescent nanotube-dicoronylene hybrids

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Luminescent nanotube hybrids were prepared by sublimation of coronene [1] on single- and multiwalled nanotubes with various diameter distribution. Samples were investigated by Raman, ATR infrared, photoluminescence spectroscopy and transmission electron microscopy. Coronene molecules were adsorbed on the nanotube surface in all samples, and were encapsulated, as well, in those that had large enough inner cavity. Though the sublimation temperature was low enough to prevent the gas phase dimerization of coronene molecules, and solid state reaction is prohibited by the crystal structure, we observed dicoronylene formation both in the inner cavity and on the surface of the nanotubes. Since the dicoronylene molecules are almost insoluble in most solvents, the coronene excess can be washed off with toluene without removing the adsorbed dicoronylene from the surface of the nanotubes. These hybrids emit green luminescence upon excitation with UV light when dispersed. We observed an enhancement of the Raman signal of the adsorbed dicoronylene molecules caused by the proximity of the nanotube surface.

[1] Okazaki et al., *Angew. Chem. Int. Ed.* 2011, 50, 4853–4857

MON 13

X-ray absorption and magnetic circular dichroism of ferrocene filled single-walled carbon nanotubes

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Changes in the nature of the magnetic state in metal filled single-walled carbon nanotubes were traced by X-ray absorption spectroscopy (XAS) and magnetic circular dichroism (XMCD). Metallic and semiconducting single-walled carbon nanotubes filled with ferrocene were measured in different conditions of temperature and magnetic field. No significant differences were found in the absorption spectra of the metallicity sorted filled carbon nanotubes. In-situ annealing process was performed on the samples and Fe nanoparticles were proved to be formed inside the nanotubes by XAS. XMCD signal becomes evident with the application of a magnetic field even at room temperature after annealing. The paramagnetic behaviour of Fe chains inside the nanotubes is also notice from the magnetic field dependent XMCD measurements. We acknowledge the BESSY II facilities and the technical assistance of the staff members. This work was supported by the Austrian Science Funds (FWF), project P621333-N20, and receiving funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n. 226716.

MON 14

Field-effect tunneling transistor based on vertical graphene heterostructures

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We report a bipolar field effect tunneling transistor that exploits to advantage

the low density of states in graphene and its one atomic layer thickness. Our proof-of-concept devices are graphene heterostructures with atomically thin boron nitride acting as a tunnel barrier. They exhibit room temperature switching ratios ≈ 50 , a value that can be enhanced further by optimizing the device structure. These devices have potential for high frequency operation and large scale integration.

MON 15

Superconducting MoN nanowires: synthesis, magnetic and transport measurements

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We report the synthesis and characterisation of novel superconducting molybdenum nitride nanowires using an efficient two-step synthetic route. We transform $\text{Mo}_6\text{S}_9-x\text{I}_x$ nanowires by annealing in ammonia-argon atmosphere. The morphology and orientation of starting MoSI material are preserved, thus enabling us to obtain thin MoN nanowires for the first time. Two types of nanowires are prepared, one with a typical diameter of 150-300 nm and length up to 10 μm and the second with a diameter from 30 to 50 nm and length of 2 μm . XRD, optical absorption, SEM with WDS, and TEM were used to characterize the MoSI precursor and the resulting MoN nanowires. SQUID measurements have verified the superconductivity of these nanowires at low temperatures. Roughly 10 % of the thick material produced undergoes a superconducting transition below 12 K. Conductivity of thicker bundles is in the range of 800-1000 S/m at room temperature. Temperature dependence of the nanowire conductivity measurements shows similar behaviour as the bulk δ -MoN. This novel superconductive nanomaterial offers a wide range of possible applications in the field of nanoelectronics.

MON 16

Development of CdS quantum dots on the surface of carbon nanotubes

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CdS nucleation and growth on the surface of carbon nanotubes (CNTs) have been achieved from water solution of CdCl_2 , thiourea, and ammonia. We experimentally studied effect of CNT annealing in an inert atmosphere on the size of CdS quantum dots. It was found that CdS nanoparticles are formed on the surface of as-prepared CNTs at room temperature during 1 min. The smallest detected size of the CdS nanoparticles is 8 nm. Development of CdS nanoparticles on CNTs, annealed at

1000C in an argon flow during 1 h, was found to require at least 5 min. The chemical state of sulfur and cadmium in the nanoparticles grown on as prepared CNTs and those after annealing was compared using X-ray photoelectron spectroscopy. The observed easier formation of CdS nanoparticles on poor graphitized CNT walls was explained based on the first-principles calculations of interaction of complexes $[\text{Cd}(\text{NH}_3)_3\text{SC}(\text{NH}_2)_2]^{2+}$ and $[\text{Cd}(\text{NH}_3)_3(\text{SH})]^+$ with the graphitic fragment. It was found that attachment of complexes is possible only near defect sites in the graphite network and the most effective nucleation of CdS is expected in the case of the $[\text{Cd}(\text{NH}_3)_2(\text{SH})]^+$ complex attachment.

MON 17

Charge-Density Wave and Superconducting Dome in TiSe₂ from Electron-Phonon Interaction

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At low temperature TiSe₂ undergoes a charge-density wave instability. Superconductivity is stabilized either by pressure or by Cu intercalation. We show [1] that the pressure phase diagram of TiSe₂ is well described by first-principles calculations. At pressures smaller than 4 GPa charge-density wave ordering occurs, in agreement with experiments. At larger pressures the disappearing of the charge-density wave is due to a stiffening of the short-range force constants and not to the variation of nesting with pressure. This suggests a common origin of the charge density waves instability in transition metal dichalcogenides, as also demonstrated by first principles calculations on bulk and few layers NbSe₂ [2]. In TiSe₂, the behavior of T_c as a function of pressure is entirely determined by the electron-phonon interaction without need of invoking excitonic mechanisms. Our work demonstrates that phase diagrams with competing orders and a superconducting dome are also obtained in the framework of the electron-phonon interaction.

[1] M. Calandra and F. Mauri, PRL 106, 196406 (2011)

[2] M. Calandra, I. I. Mazin and F. Mauri, PRB 80, 241108(R) (2009)

MON 18

Transport in graphene with superlattices

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An important parameter that defines the range of electronic phenomena accessible in graphene experiments is its carrier mobility (μ). There are three main candidates which limit μ : charged impurities, random strain and resonant (strong) scatterers (RS). RS have been observed recently in graphene with hydrogen adsorbates and vacancies. In addition, RS may also be conveniently induced by metallic islands

deposited on the graphene surface. In this case, the strength of the impurity scattering can be controlled by a local external gate. Moreover, these impurities can be arranged on graphene in a periodic pattern, i.e. forming a superlattice (SL). The conductivity in this type of structures is predicted to change depending on the superlattice structural parameters. Furthermore, if SLs are fabricated with magnetic impurities, an enhancement of spin polarization and magneto-resistance are expected. In our study metallic dot-patterns are defined on graphene. Transport measurements under external magnetic field are undertaken to detect variations in the resistance and magneto-resistance imposed by the superlattice.

MON 19

Dimensionality in nanocarbon-based thermoelectric meta-structures

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For nanotube-based polymer blends, a thermoelectric figure of merit $ZT \sim 0.02$ to 0.05 can be achieved based upon the simple premise that the nanotubes conduct charge by hopping while nanotube-nanotube junctions block the flow of heat. Surprisingly, much larger thermovoltages and power factors can be achieved from such materials when they are formed into composite meta-structures, in which heterogeneous arrays of percolating nanocarbon allotropes are alternated with a thermally insulating polymer layer. We describe the fabrication of such architectures using ink-jet printing. Such modules using doped carbon nanotubes, is well described by standard models, with the individual layers adding linearly to the overall power output. However, the analogous modules printed from doped graphene sheets can not be explained in the same manner. In this work we explore the detailed experimental differences between the thermoelectric response of graphene and nanotube composite systems. We then examine the role of “space filling” or “fractal dimensionality” in the graphene-composite system and introduce a model to understand the theoretical limits that may exist.

MON 20

Synthesis of Carbon Nanostructures grown on Aligned ZnO Nanorods

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Novel synthesis techniques allow to control the architecture of many different materials at nanoscale and allow the growth of many hybrid nanostructures suitable for many technological applications, spanning from sensor to supercapacitors. By combining in situ X-ray photoemission spectroscopy, ex situ scanning electron microscopy and Raman spectroscopy, we show that chemical vapour deposition (CVD), done on vertically aligned ZnO nanorods (NRs), is able to synthesize different carbon nanostructures, whose morphology is driven by the ZnO NRs and whose dimensions and structure change as a function of the CVD temperature. The carbon nanostructures span from amorphous carbon cups, covering the ZnO NRs, to high density, short (≈ 100 -200nm) carbon nanotubes (CNTs) nucleating on the ZnO NRs, which result to be partially etched in the process temperature range 630-740°C. The ZnO NRs are completely etched when CVD is done at higher temperature, leaving only CNTs preferentially aligned along the location of the pristine NRs. This simple method can enable to produce with high control different architectures of nanostructured carbon, using cheap templates (ZnO) and industrial process (CVD).

MON 21

Multifrequency Raman on graphite intercalation compounds from Stage I - Stage VI revisited

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Graphite Intercalation Compounds (GIC) with alkali-metals in between has been a field of study for decades. However their Raman response still not completely resolved because of laser induced deintercalation. In this work we performed a detailed in-situ Raman analysis under high vacuum conditions for potassium GIC from stage-1 to stage-6. A detailed Raman lineshape analysis was applied to determine the intrinsic response of stage one KC_8 compound proving that the intrinsic **G-line** of KC_8 is at 1510 cm^{-1} . From this starting point, lower intercalation stages were produced by subsequent deintercalation and reintercalation steps. In agreement with previous results we observe for stage III to VI a clear doublet in the G-line which corresponds to pristine and charged graphene layers. We found a strong and different resonance Raman behavior of the two components for the different GIC. This is supported by ab-initio results. In addition we present an accurate description of the dispersion of the 2D line for different GIC which has important implications for the analysis of pristine and doped graphene. Work supported by FWF-I377-N16, and OEAD AMADEUS PROGRAM.

MON 22**Structure and physical properties of nanoclustered graphene synthesized from C60 fullerene under high pressure and high temperature**

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C60 treatment at high-pressure (3-8 GPa)/high-temperature (1000 K) results in the fullerene cages collapse and transformation to a phase with outstanding mechanical properties. A detailed analysis of the material structure by XRD and HRTEM reveals that it is comprised of 7-15 layer graphene clusters with lateral dimension of 2-4 nanometers. Typically the layers are non-planar (corrugated) and separated by 0.36 nm. Importantly, there is a preferred orientation of the graphene planes which is probably inherited from the parent C60. Raman spectra of the nano-sized graphene clusters are similar to those of disordered sp² structure with an admixture of sp³-bonded carbon. The phase is characterized by a high hardness (up to 17 GPa), relatively low elastic modulus (up to 110 GPa), and a high elastic recovery (up to 94%). This unique combination of high hardness and elasticity determines excellent wear resistance and good antifriction properties, which may have direct implication for design of new metal-carbon composites with enhanced tribological characteristics. A structural model of C60 transformation to nanoclustered graphene is discussed.

MON 23**Electrical Transport properties of sub-20nm Germanium Nanowires**

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Recently there has been renewed interest in studying the properties of germanium due to its high electron and particularly hole mobility when compared to silicon. In this study we have investigated the basic electrical characteristics of germanium nanowires with a crystalline germanium core with a diameter down to below 20 nm and an amorphous, non-conducting shell. Nanowires grown using two different synthesis conditions have been characterised. The nanowires have been contacted by nickel and cobalt electrodes in two point and four point configuration. The value of the resistivity in the wires from both growth conditions has been found to be less than the value in bulk germanium. Differences in the shell caused by the varying synthesis conditions lead to a change in the surface states which result in changes in the transport properties being observed. These range from memristive and p-type

conduction for one growth condition to relatively low resistivity and little or no gate effect for the other growth condition. It is suggested that the latter result is due to a high density of surface states leading to doping past the Mott transition.

MON 24**Fast and efficient combustion synthesis route to produce exfoliated graphite**

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Micromechanical exfoliation produces graphene flakes from the layered material graphite. As the wet chemistry protocol, with the intermediate graphite oxide formation, is quite involving [1], we report the exploratory study on simple one-step chemical synthesis of exfoliated graphite via a combustion synthesis route. The different solid carbonates could be atomized upon reducing in solid phase [2]. The formed carbon elemental coalesced towards 1D nanocarbons. Recently, such processing was extended into the direct heterogeneous, high-pressure reduction of gaseous carbon oxides to elements (CO₂, CO) with Li, Mg, Ca, and other strong reducers in a modified calorimetric bomb [3]. The products were chemically purified. The morphology identification of produced layered carbon was done by XRD, SEM, TEM, Raman spectroscopy.

[1] M. Inagaki et al., J. Phys. Chem. of Solids, 675, 133-137 (2004)

[2] A. Dabrowska et al., Phys. Status Solidi B, 248, 2704-2707 (2011)

[3] A. Huczko et al., J. Mater. Res., in print (2011)

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MON 25**Equilibrium Torsion in Chiral Carbon Nanotubes**

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The proposal [1] of slight twist with respect to the rolled up configuration in chiral single-walled carbon nanotubes is recently numerically justified [2]. Only dynamical models supporting full helical symmetry (monomer becomes minimal repeating component) can show this effect, while standard DFT assume translational periodicity.

Here we present convincing evidence for the effect: very similar dependence of the torsion angle of the tube diameter (rapid decrease) and chiral angle within several dynamical models like pairwise harmonic potential, Brenner potential based molecular dynamics, and DFTB. Also, we give indirect justification of torsion using full DFT code SIESTA.

Accompanying change in symmetry through the parameter Q of rotation of the helical axis enables to analyze experimental observation of the effect in terms of diffraction: we singled out features of the patterns related to the torsion, and show that in narrowest nanotubes the effect can be measured.

[1] M. Damnjanović, B. Nikolić, and I. Milošević, Physical Review B 75, 033403 (2007)

[2] D. G. Vercosa et al., Physical Review B 81, 165430 (2010)

MON 26

Transport properties of graphene nanoribbons with a reduced disorder potential

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Graphene exhibits a number of unique electronic properties making it to a very promising material for future nanoelectronics. However the absence of a band gap is one of the key problems on the way to a graphene-based technology with today's electronic device concepts. By structuring graphene into narrow ribbons in the nanometer range a transport and effective energy gap can be opened. However, the gap characteristics cannot be explained by a single-particle quantum confinement picture and reproducible resonances can be observed within the entire transport gap. The origin of these effective energy gaps and the local resonances is assumed to be related with the disorder potential arising from the substrate and the edge roughness. We present electron transport measurements on lithographically defined and etched graphene nanoribbons with focus on studying the influence of the disorder potential on the transport gaps. Short treatments with hydrofluoric (HF) acid are used to change the disorder potential and result in different transport characteristics. Measurements before and after the HF dip on the very same samples verify the effect on the disorder potential.

MON 27

Chemical functionalization of carbon nanotubes by coating with titanium.

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The study of the carbon-metal interaction is an important task for application of carbon materials in electronic devices and metal matrix composites. In particular, a low ohmic contact through formation titanium carbide is required for nanoelectronics. Further, the metal matrix composites with reinforced mechanical properties and reduced thermal expansion might lead to the extended medical applications

implementing biocompatibility of titanium. However, the carbon nanotubes (CNT) are not easily wetted by molten metal. Generally, a thin titanium layer may act as a carbon-metal interface improving the wettability of CNT by any others metals. In this study, we investigated the possibility of chemical vapor deposition of titanium on CNT using TiCl_4 as precursor and H_2 gas as a reducing agent in a protective atmosphere of argon. In a typical experiment, the TiCl_4 was blown over the nanotube sample placed in a quartz tube and heated in furnace at 873 K for 1h. The SEM images of the Ti coated nanotubes show no apparent change in morphology in comparison to the starting CNT material. The presence of titanium is confirmed by the EDX spectrum.

MON 28

Enhanced wetting of ALD grown dielectrics on CVD graphene

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The growth of *nm*-thick dielectrics on graphene could further unlock graphene's potential for applications such as RF FET (thin high-k gate oxides for optimal channel control¹), lateral spin valves (tunnel barriers for spin injection²) or pseudo-spin FET (tunnel barriers to couple two stacked sheets³). Interestingly, continuous *1nm* films have already been grown by sputtering². While atomic layer deposition (ALD) could ensure further compatibility with monolayer graphene, inorganic⁴ or organic⁵ seed layers have been needed to grow continuous films $\leq 10\text{nm}$. We will present experimental data focusing on $\leq 10\text{nm}$ high-k dielectric films (Al_2O_3 , HfO_2) grown by direct ALD on different graphene-like materials (CVD-grown, graphite, graphene/ SiO_2). Their wettings are compared and a strong enhancement of the wetting is reported on large scale high quality CVD graphene. This phenomenon allows further down-scaling of ALD dielectrics on graphene.

¹F. Schwierz, Nat. Nano. 5, 487, 2010

²B. Dlubak et al., APL 97, 092502, 2010

³S Banerjee et al., IEEE Elect. Dev. Lett. 30, 158, 2009

⁴J Robinson et al., ACS nano 4, 2667, 2010

⁵I. Meric et al., Nano Lett. 11, 1093, 2011

MON 29

Nanopore Graphene-based Electronic Devices

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A new generation of solid state nanopore devices with enhanced biomolecule sensitivity is possible by incorporating more complex device fabrication near the pore. We developed various micro and nano fabricated device designs to take advantage of the thickness and electronic properties of graphene. In order to identify sources of

current leakage – a necessary step in understanding device functionality – we study the electrochemistry of the material components of the devices in KCl solution. We measure DNA translocations through a variety of layered pores that correspond with potential device configurations and find similar ionic results to traditional silicon nitride nanopores. These findings suggest the proposed configurations are viable as nanopore sensing devices.

MON 30

Scattering of electrons with acoustic phonons in single-walled carbon nanotubes

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Using photoluminescence excitation spectroscopy, we determine the first two transition energies for carbon nanotubes (CNTs) in solution and free standing, vertically aligned CNTs. We observe considerable energy shifts depending on dielectric screening and Coulomb interaction between these two samples and explain them by microscopic calculations based on density matrix formalism. Combining experiment and theory, we determine the dielectric background constant of the CNT-forest and CNT-solution to be 1.3 ± 0.1 and 1.8 ± 0.1 , respectively.

Further, using the CNT-solution sample in a joint study of two-color pump-probe experiments and microscopic calculations, we extract, both experimentally and theoretically, a picosecond carrier relaxation dynamics, and ascribe it to the intraband scattering of excited carriers with acoustic phonons. The calculated picosecond relaxation times show a decrease for smaller tube diameters. The best agreement between experiment and theory is obtained for the (8,7) nanotubes with the largest investigated diameter and chiral angle for which the applied zone-folded tight-binding wavefunctions are a good approximation.

MON 31

Transport in coupled graphene-nanotube based quantum devices

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Carbon nanomaterials, such as carbon nanotubes (CNTs) and graphene, both exhibiting unique electronic and mechanical properties are very promising materials

for future nanoelectronic applications. The absence of the hyperfine field in C12 enriched carbon materials makes CNTs and graphene particularly interesting for hosting quantum dots (QDs) which potentially allow the realization of spin-qubits with long coherence times. Here, we present the fabrication and electrical characterization of all carbon devices based on both, graphene as well as CNTs. In particular we show a device in which the charge state of a CNT QD can be detected by measuring the conductance through a 100 nm wide and 150nm distant graphene nanoribbon. Changes of the conductance of up to 20% are obtained at single charging events. Furthermore, we present a CNT QD where the source and drain leads consist of single- and bi-layer graphene. Charging energies of 1-1.5 meV of the investigated QD, extracted from Coulomb diamond measurements are in good agreement with the CNT length in between the leads of 1.2 μm and let us conclude that a tunnel barrier is present at the interface of both carbon allotropes.

MON 32

Efficient energy transfer in perylene-nanotube complexes

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Carbon nanotubes are interesting for biomedical applications because they emit in the IR part of the spectrum; establishing nanotube-adsorbant energy transfer complexes in aqueous solution is thus a key step towards the complex non-covalent functionalization of nanotubes in biocompatible environments. We demonstrate direct energy transfer in perylene-imido-diester nanotube complexes in water: upon excitation of the adsorbed perylene unit we observe an emission from the carbon nanotubes, which indicates a successful excitation transfer. The efficiency of the indirect excitation via the adsorbant is of the same order of magnitude as the direct excitation of the nanotubes. Furthermore the perylene-imido-diester compound simultaneously serves as a surfactant for the nanotubes, obliterating the need for a supplementary surfactant. We thus created a self-sufficient excitation transfer complex which is stable in an aqueous medium over many months.

MON 33

Study of nanoparticle formation using the cyclic method of catalyst design

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Forests need to have the highest density to use carbon nanotubes as vias and interconnects in integrated circuits and thermal interface materials. The areal density of nanotube forests can be dramatically increased using our catalyst preparation technique, i.e., cycles of deposition and annealing of ultra-thin metal films followed by nanoparticle immobilisation.[1] In this work, we use systematic cross-section trans-

mission electron microscopy after each cycle to show how the density of the catalyst nanoparticles increases. We prove that the layers of metal catalyst, subsequently deposited after previous annealing, sit on the uncovered areas of the support, which, after annealing, restructure into nanoparticles increasing their density but not significantly their size. These nanoparticles lead to close-packed, high-density nanotube forests. The areal densities of the forests are re-assessed by employing the weight gain method; we can confirm nanotube areal densities of the order of 10^{13} cm^{-2} . Further density increase, close to the limit of a fully dense forest (10^{14} cm^{-2}) is achievable by reducing nanotube diameter.

[1] S. Esconjauregui et al. ACS Nano 4, 7431 (2010).

MON 34

Ab-initio investigation of regular vacancies influence on elastic and magnetic properties of graphene and graphene-like structures BN and SiC

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Influence of regular monovacancies on magnetic and elastic properties of graphene and BN and SiC structures have been calculated in the frame of DFT-GGA formalism by VASP package. We show that increasing of vacancies concentration in the graphene leads to monotonic decreasing of elastic modulus from the value of defect-free graphene modulus ($\sim 1 \text{ TPa}$) to 0.8 TPa . Also the influence of graphene's vacancies as well as of both vacancy kinds (B and N in the BN structure, Si and C in the SiC structure) on magnetic properties is investigated. It is shown that C vacancies in the SiC structure lead to a paramagnetic state, but in all other cases the magnetic states are essentially lower than the paramagnetic state. The increasing distance between vacancies from 7.4 \AA to 19.6 \AA leads to change of antiferromagnetic order to ferromagnetic one. At that the ferromagnetic-antiferromagnetic energy splitting is extremely low ($\sim 10^{-4} \div 10^{-3} \text{ eV}$) for the vacancies in the graphene and N vacancies in the BN structure. At distances between vacancies more than 12.3 \AA the ferromagnetic-antiferromagnetic energy splitting becomes again very low in the all structures

MON 35

Water assisted CVD synthesis of millimeter-long and aligned coiled carbon nanotube forest

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Coiled carbon nanotubes possess unique properties of helix, chirality and nonlinear mechanical behavior. It attracts great interests in the synthesis, growth mechanisms and application developments. CCNTs have potential applications in nano-electromechanical devices, composite reinforcements, etc. Until now millimeter-long array of coiled carbon nanotubes have never been produced. The aligned coiled carbon nanotube forests were produced catalytically by water assisted CVD of ethylene. After deposition on an iron-coated silicon substrate the structure of a helix-shaped multiwalled nanotubes offer a densely packed aligned nanospring product. The challenges in this field include delicate control of parameters in structure, now we are going to present the parametric study which helped us to optimize the growth process.

MON 36**The role of nanotubes in carbon nanotube-silicon heterojunction solar cells**

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Currently there exists a great interest in finding alternative semiconductor materials for use in photovoltaic architectures. One material with great potential is the carbon nanotube (CNT). Towards this goal CNTs have been combined with the well understood, model semiconductor material, silicon, in a so-called nanotube-semiconductor heterojunction (NSH) solar cell. This device is similar to that of a p-n junction crystalline silicon solar cell with the exception that the p-type emitter layer is replaced by a thin film of CNTs. Currently the literature consists of several examples of such solar cells, however it remains unclear if such cells operate as a typical p-n junction solar cell or a Schottky junction solar cell, or the closely related metal insulator semiconductor solar cell. In this work we have employed chirality sorted single-walled CNTs (SWCNT), prepared by size exclusion chromatography to create various NSH solar cells. Upon comparison of wavelength resolved external quantum efficiencies and UV-Vis absorption spectra/photoluminescence maps of the chirality sorted SWCNTs, insights into the role SWCNTs play in the operation of NSH solar cells have been gained.

MON 37**Phase transitions in $C_{60}\cdot C_8H_8$ induced by hydrostatic pressure**

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High-pressure infrared transmission measurements up to 9.5 GPa were carried out on the rotor-stator molecular cocrystal $C_{60}\cdot C_8H_8$ using helium as hydrostatic pressure transmitting medium, which can intercalate into the $C_{60}\cdot C_8H_8$ lattice. The goal of this study was to investigate the pressure effects and the effect of the intercalation of helium in the $C_{60}\cdot C_8H_8$ lattice. The pressure-induced shifts of the vibrational modes of $C_{60}\cdot C_8H_8$ show an anomaly at around 3 GPa. The anomaly is observed at higher pressure compared to the earlier high-pressure studies [1] on $C_{60}\cdot C_8H_8$, probably due to the intercalation of helium in the $C_{60}\cdot C_8H_8$ lattice or the better hydrostaticity. This anomaly can be interpreted in terms of the orientational ordering transition of fullerene molecules accompanied by a change in the crystal symmetry of $C_{60}\cdot C_8H_8$, causing the splitting of the vibrational modes.

[1] K. Thirunavukkuarasu et al., J. Phys. Chem. C **112**, 17525 (2008).

MON 38**Strain-induced inversion symmetry breaking in Bernal-stacked bilayer graphene**

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We present a systematic uniaxial deformation Raman study of several bilayer graphene samples embedded in a polymer matrix, using laser energies from the visible to the near-IR range. Our experimental data show that strain directly influences the double resonance bands, while the $2D_{11}$ component is more sensitive to the induced deformations. In terms of the mechanical stability, we observed that the

interface failure or slippage of the bilayer occurs at lower tension levels compared to the monolayer part of the same flake. Additionally, the Bernal-stacked two layers fully embedded in a matrix are locally susceptible to non-uniform strain field components, which induce a breaking of the bilayer inversion symmetry. This in turn leads to the activation of the infrared E_u mode and the appearance of a single broad 2D band component. The results can be explained considering the band-gap opening, as proposed by recent theoretical predictions. Further work towards a control, at a larger scale, of the strains applied independently to each of the two layers is needed to confirm the viability and the potential of such a mechanism.

MON 39**Synthesis of novel thiophene-phenylene oligomer derivatives with dibenzothiophene-S,S-dioxide core for applications to organic solar cells**

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Thiophene-containing oligomers with well-defined structures and monodispersed chain lengths, are easily modified by the introduction of a variety of functional groups into the aromatic backbone or through thienyl sulfur functionalization, and have attracted a great attention for their possible use in organic electronics such as organic solar cells (OSCs). Thiophene-phenylene oligomers are promising electron-donor semiconducting materials with improved oxidation stability. However, there is no report about the synthesis of thiophene-phenylene oligomer derivatives containing dibenzothiophene-S,S-dioxide moiety and their applications in OSCs. In this study, we newly synthesized donor-acceptor-donor thiophene-containing oligomers by introducing dibenzothiophene-S,S-dioxide groups with electron-acceptor character into the frameworks of thiophene-phenylene oligomers via co-oligomerization [1]. New oligomers were characterized by UV-vis absorption and photoluminescence spectroscopy, cyclic voltammetry. It was found that new oligomers are valuable electron donors and can be used in OSCs. The detailed characteristics will be discussed. [1] Z. Duan et al. Chem. Lett. (2012)

MON 40**De-hydrogenation and remanent magnetization of metalated 2H-tetraphenylporphyrins on 3d magnetic substrates**

Andrea Goldoni¹, Giovanni Di Santo¹, Carla Castellarin-Cudia^{1,2}, Luca Floreano¹, Alberto Verdini², Albano Cossaro², Elena Magnano², Federica Bondino², Stephan

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One monolayer of 2H-Tetra-Phenyl-Porphyrins (2H-TPP) on Ag(111) annealed at $525 < T < 600$ K shows irreversible chemical modifications. Selective carbon dehydrogenations, the formation of new aryl-aryl bonds between phenyl substituents and the macrocycle, as well as the rotation of the phenyl rings in a flat conformation are observed by NEXAFS and STM and theoretically explained using DFT calculations. Moreover, we show that depositing one monolayer of 2H-TPP on Fe and Ni films at room temperature, the macrocycle binds directly to an adatom of the metallic substrates and metalates the porphyrin. We investigate the in-situ-prepared monolayer and sub-monolayer of metalated Mn-TPP deposited on 1 ML of metalated Fe-TPP obtained on a film of Fe/Cu(110) with the above procedure. For the adsorbed metalated Mn-TPP molecules we will study the magnetic properties using NEXAFS and XMCD measurements, in combination with theoretical calculations of the electronic structure. We will demonstrate that the easy axis of magnetization is reversed in the second layer made of Mn-TPP from the in plane Fe magnetization of the first metalated Fe-TPP layer deposited on Fe/Cu(110).

MON 41

Covalent and ionic functionalization of quasi-free-standing graphene

Alexander Grueneis^{1,2}, Danny Haberer¹, Luca Petaccia³, Alexei Nefedov⁴, Dima Usachov⁵, Denis Vyalikh⁶, Alessio Paris⁷, Nicolay Verbitskyi⁸

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Here we show by photoemission spectroscopy that the interaction of graphene with foreign atoms can tailor its electronic properties and induce band gaps, additional electronic states and charge transfer to graphene. We modify graphene covalently by hydrogenation, deuteration, incorporation of nitrogen atoms and induce ionic functionalization by deposition of alkali metal atoms onto graphene. Regarding covalently doped graphene we report (1) a strong kinetic isotope effect for the chemisorption kinetics of deuterium and (2) a conversion from pyridinic nitrogen to graphitic nitrogen impurities. Regarding ionic doping, we carefully analyze graphene's spectral function in order to extract the full momentum dependent Eliashberg

function of graphene from angle-resolved photoemission spectroscopy (ARPES). The Eliashberg function is the central quantity in a coupled electron-phonon system and its determination unravels the contribution of each phonon mode to the "kink" feature frequently observed by ARPES of heavily doped graphene and graphite intercalation compounds.

MON 42

Light energy conversion by photosynthetic reaction center linked specifically to carbon nanotubes

Kata Hajdu¹, Balázs Réti², Zoltán Németh², Krisztina Nagy³, György Váró³, László Forró⁴, Klára Hernádi², László Nagy¹

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Reaction center (RC) is one of the most important proteins converting light energy into chemical potential in the photosynthetic membrane assuring conditions for carbon reduction in cells. It is possible to immobilize the purified RC to different carrier matrices in order to use the excited electrons for any wanted redox reaction. The interaction between single-walled carbon nanotubes (SWNT) and photosynthetic reaction centers purified from purple bacterium *Rhodobacter sphaeroides* R-26 has already been investigated. Structural and functional studies clearly testify that the reaction center protein can be attached effectively to the nanotubes. It is expected that chemical attachment of the reaction centre assures a stronger linkage between the two materials as compared to the physical binding. Different functionalized (like amine-functionalization, silicon-coverage) carbon nanotubes are used to bind the RC more efficiently. Kinetic measurements show that the RC preserves its activity on the nanotube surface for a longer time. The special electronic properties of the SWNT/protein complexes open the possibility for several applications, e.g. in microelectronics or energy conversion.

MON 43

Change in nanotube Fermi energy upon deposition: A Raman scattering study

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Raman spectroscopy yields plenty of structural information on single-walled carbon nanotubes. The shape and the spectral position of the phonon modes around 1590 cm^{-1} , called G or high energy modes (HEMs), may indicate the presence of metallic carbon nanotubes due to phonon softening by a Peierls-like mechanism.[1] We find that the HEMs of a chirality enriched sample[2] in solution resemble those of a semiconducting spectrum, while upon deposition on silicon the spectra appear to be metallic. Radial breathing mode spectra confirm that the HEMs arise from metallic nanotubes in both cases, hereby excluding that shifts in transition energy upon deposition give rise to different phonon line shapes. Instead, we explain our results in terms of Fermi energy shifts, which influence the HEM line shape of metallic tubes. This result is relevant for the identification of metallic tubes from the HEM line shapes through Raman scattering, a common and speedy experimental approach.

[1] O. Dubay et al., Phonon Softening in Metallic Nanotubes by a Peierls-like Mechanism, Phys. Rev. Lett. 88, 235506 (2002) [2] C. Blum et al., Selective Bundling of Zigzag Single-Walled Carbon Nanotubes, ACS Nano 5, 2847-2854 (2011)

MON 44

Synthesis and comparative characterization of SnO₂-MWNT nanocomposite materials

Klára Hernádi¹, Zoltan Pallai¹, Vladimir M. Aroutiounian², Arsen Z. Adamyan², Emma A. Khachaturyan², Zaven N. Adamyan², Arnaud Magrez³, László Forró³, Zoltán Németh¹

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Multi-walled carbon nanotubes (MWNTs) were successfully coated with tin-dioxide (SnO₂) nanoparticles by either hydrothermal process using $\text{SnCl}_2 \times 2\text{H}_2\text{O}$ or sol-gel method using $\text{SnCl}_4 \times 5\text{H}_2\text{O}$ as precursor under different solvent conditions. The obtained nanocomposites had the component mass ratio of 1:4, 1:8 and 1:50, respectively. The as-prepared SnO₂-MWNTs nanocomposites were characterized in detail using transmission and scanning electron microscopy (TEM, SEM), Raman microscopy (DXR Raman) and X-ray powder diffraction (XRD) technique. The aim of this work is to present a simple one-step controllable method, which provides SnO₂/MWNT composite materials the proper morphology (continuous coating, thickness, etc.). These materials are suitable for further applications in both gas sensor technology and photocatalysis.

MON 45**Towards Flexible, Conducting and Transparent Coatings: Carbon Nanotube-Aluminium doped Zinc Oxide Composites**

Endre Horváth¹, Iwan Thomas¹, Quentin Python¹, Jacim Jacimovic¹, Rita Smajda¹, László Forró¹, Arnaud Magrez¹

¹Ecole Polytechnique Federale de Lausanne, Switzerland

Transparent Conducting Oxides (TCOs) are fundamental to several modern-day technologies including touch screens, flat-panel displays and solar cells. Traditionally, doped metal oxides have played this role, most commonly indium-doped tin oxide (ITO). As well as being rare and expensive, ITO is brittle leading to easily damaged films. We have developed novel indium-free composite materials by sputtering aluminium doped ZnO (AZO) on a transparent film of millimetre long CNTs. The conductivity of the composites increased with the AZO thickness and their transparency decreased with CNT thickness. Best films exhibited a sheet resistance of 100Ω/sq and a transparency for visible light of about 75%. The flexibility of these films has been tested when deposited on PET substrate. The presence of a flexible CNTs mesh underneath the AZO film acts as a conductive path between the particles when cracks form while the film is bent. As a consequence the resistance only increases to 1.5 R₀ when the film is bent and after 200 bending cycles the resistance (R₂₀₀) increased only by a factor of 2. This study shows that these AZO and CNTs-based films are very promising for flexible applications.

MON 46**Assessment of the Cellular Toxicity of Graphene Oxide In vitro**

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Graphene-based materials will have a profound impact on a broad range of applications including catalysis, electronics, renewable energy and composites. Due to the versatility of the production methods and the relative ease of functionalization, it is expected that the number of graphene-based derivatives will significantly increase in the near future. It is therefore primordial to systematically test these materials for their biocompatibility and safety for industrial and biomedical use and redesign them, if necessary to be safe with respect to cytotoxicity and more importantly carcinogenesis of either lung tumors or mesotheliomas. However, the studies devoted to the putative adverse health effects of graphene materials are hugely underrepresented in the current scientific literature. We performed cell viability studies on lung epithelial and macrophage cells exposed to graphene-oxide (GO). Our experimental results demonstrate a mild acute cytotoxic action of GO

with a cell survival $\geq 80\%$, a dose-dependent impact on the mitochondrial activity of the cells and a cell-type and dose-dependent induction of cell death including apoptotic and necrotic mechanisms.

MON 47**RF plasma: emission spectroscopy diagnostics and CVD process of carbide and carbon nanofilms growth**

Andrzej Huczko¹, Magdalena Kurcz¹, Hubert Lange¹

¹Department of Chemistry, Warsaw University, Warsaw

RF inductively coupled low-temperature plasma can be an interesting environment for growing not only thin films but even graphene layers. Process variables, such as: discharge power, or chamber pressure allows us to control a structure and a stoichiometry of a product. SiC is an interesting material, which is used not only as a wear-resistant coating but also as a high-temperature, wide band-gap semiconductor. Thus, it has been extensively studied and much attention has been focused on methods of its growth. A systematic study of the influence of selected parameters of plasma process on a growth of SixCy thin films is presented. For comparison, thin pure carbon/graphite films have been also produced. The films were characterized by various methods to investigate the effects of the process parameters on their growth. Optical emission spectroscopy provides an excellent means of understanding the basic transformations of excited reactants. Thus, the special attention was paid to plasma diagnostic.

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MON 48**Raman scattering measurements of electronically separated SWNTs**

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In our contribution, we present results of Raman scattering experiments on electronically separated single-walled carbon nanotubes. The spectra were excited with laser lines across the entire visible range. For semiconducting nanotubes, we found a couple of strongly dispersive (more than $100 \text{ cm}^{-1}/\text{eV}$) modes at about 400 cm^{-1} . In contrast to the D line, these modes reveal a negative dispersion, e.g. their frequency decreases with the increasing laser energy.

We also recorded spectra of HNO₃-doped samples. The Raman response is markedly different depending on the electronic character of the sample. For semiconducting

nanotubes, doping leads to an overall decrease of the intensity of Raman lines. The same holds for phonon modes of metallic tubes. For the metallic tubes in addition a broad band between 1000 and 4000 cm^{-1} develops in the spectra when excited with red laser lines. Qualitatively, the feature resembles a broad band observed in spectra of Li-doped graphite as it was reported some decades ago. Possible origins of the band are discussed.

MON 49

Carbon Nanotube Bundles Self-Assembled in double helix microstructures

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Carbon nanotubes (CNTs) offer unique opportunities for producing new materials due to the possibility of engineering their structure at the molecular level and controlling their assembly. Self-assembling coiled bundles of CNTs would take advantage of CNTs' mechanical properties and the also of the properties emerging from the coiled shape in itself (i.e. high axial stiffness, strain to failure and large energy absorption by mechanical deformation). We report the synthesis and structural characterization of novel carbon materials; self-assembled double-helices of CNTs bundles [1]. These are catalytically grown by Fe nanoparticles bonded to SiO_x microparticles, similarly than for coiled bundles of single-walled CNTs [2]. Differently than in most of previous works on coiled carbon microstructures [3], where coils are supposed to be achieved by introducing curvature on the CNT/fibres building blocks, we present a growth model relaying on a microstructural instability during the growth. Finally possible applications are suggested. [1]F. Cervantes-Sodi, et.al. Submitted(2012). [2]Q. Zhang, et.al. Angew. Chem. Int. Ed. 49, 3642(2010). [3]S. Motojima et.al. Appl. Phys. Lett. 56, 321(1990).

MON 50**Carrier control of SWCNT thin film transistors by molecular encapsulations**

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Previous works demonstrated that semiconducting single-wall carbon nanotubes (s-SWCNTs) can be used as a high-mobility channel of thin film transistor (TFT). For the fabrication of complementary TFTs as a building block of logic circuits, however, carrier control of s-SWCNTs is essential. It is well known that the p-type TFT can be naturally obtained by hole injection from oxygen molecules adsorbed on to the s-SWCNT wall. However, it was not easy to prepare an air stable n-type TFT. In this work, we prepared ferrocene encapsulated s-SWCNTs and used it as an n-type channel. High-yield filling of ferrocene molecules and accompanying electron injection was confirmed by Raman, optical absorption, and photoluminescence spectra. Then transport properties of back-gated TFTs were measured under vacuum (10^{-4} Torr). They clearly exhibited n-type behaviors while undoped TFT showed normal ambipolar behavior. To our knowledge, this result is the first evidence that molecular encapsulated s-SWCNTs can be used as an n-type channel under vacuum.

MON 51**Low temperature diamond growth by linear antenna plasma CVD over large areas**

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Recently, there is a great effort to increase the deposition area and decrease the process temperature for diamond CVD deposition which will enlarge its applications including the CVD growth on temperature sensitive substrates. In this work we reported on the large area and low temperature diamond growth by pulsed linear antenna microwave plasma system. The influence of substrate temperature varied from 250 °C to 700 °C, as controlled by the table heater and/or by MW power, was studied. It was observed that the growth rate, film morphology and diamond to non-diamond phases (sp^3/sp^2 carbon bonds) are significantly influenced by the growth temperature, as confirmed by SEM and Raman measurements. The surface chemistry and growth processes were studied in terms of activation energies

(E_a) from Arrhenius plots. The activation energies of growth processes were very low ($3\div 5$ kcal/mol) indicating an energetically favourable growth process from the $\text{CO}_2\text{-CH}_4\text{-H}_2$ gas mixture as comparing to the standard $\text{CH}_4\text{-H}_2$ gas chemistry ($26\div 30$ kcal/mol). In addition, high re-nucleation rate was observed for the low temperature process.

MON 52

Field and temperature dependence of conductivity in carbon-based materials

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The conductance of conducting polymer nanofibres, carbon nanotube networks and other materials with nanoscale structure shows a characteristic increase as bias voltage increases [1]. Chemically reduced graphene oxide also shows a strong increase of conductance with bias voltage, especially at low temperature [2]. We investigate the mechanisms responsible for this electric field dependence and the correlation with the temperature dependence of conductance, which in the presence of disorder often follows variable-range hopping or fluctuation-assisted tunnelling behaviour [3,4].

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MON 53

Raman spectroscopy of isotopically engineered two layer graphene

Martin Kalbac^{1,3}, Ladislav Kavan¹, Hootan Farhat², Jing Kong³, Mildred S. Dresselhaus^{3,4}

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A detailed understanding of graphene properties both in its neutral and doped states is an important prerequisite for applications of this new material in electronic devices. In general, doping of graphene leads to a shift of the Fermi level and

therefore it represents a simple way to control graphene electrical and optical properties. The doping can be realized chemically, electrochemically or by electrostatic charging. The electrochemical doping can be easily controlled and it allows to reach relatively high doping levels of graphene. In our study we used electrochemical doping to study the influence of charge on one-layer and two-layer graphene. In the case of two layer graphene we prepared isotopically engineered sample where one layer of graphene was formed by ^{13}C while the second layer from ^{12}C . This approach allowed us to monitor charge distribution between the top and bottom layer which is very important for prospective application of two layer graphene in electronic devices like bilayer pseudospin field effect transistor. Reference: M. Kalbac, H. Farhat, J. Kong, P. Janda, L. Kavan, and M. S. Dresselhaus: *Nanoletters*, 11(5), 1957-1963 (2011).

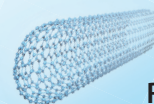
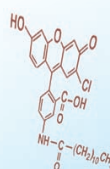
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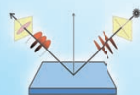


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$$\rho = I_p/I_s = \tan \Psi e^{i\Delta}$$



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Carbon nanotube spectroscopy

Tuesday, March 6th

- 08:30 – 09:00 **T. Heinz, New York**
Probing Interactions in Single- and Few-Layer Graphene by Optical Spectroscopy
- 09:00 – 09:30 **G. Cancado, Belo Horizonte**
Raman characterization of nanocarbons
- 09:30 – 10:00 **S. Berciaud, Strasbourg**
Intrinsic optical properties of free-standing carbon nanotubes and graphene monolayers
- 10:00 – 10:30 **Coffee break**
- 10:30 – 11:00 **R. Narula, Berlin**
Dominant phonon wavevectors and strain-induced splitting of the 2D Raman mode of graphene
- 11:00 – 11:30 **L. Wirtz, Luxembourg**
Theory of Raman spectroscopy of graphene on different substrates
- 11:30 – 12:00 **J. Maultzsch, Berlin**
Double-resonant Raman modes in few-layer graphene
- 12:00 – 17:00 **Mini-Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **A. Chernov, Vienna**
ESR from fully metal – semiconductor separated SWCNTs
- 19:00 – 19:30 **G. Lanzani, Milan**
Ultrafast confocal microscopy and CT dynamics
- 19:30 – 20:00 **T. Pichler, Vienna**
Electronic transport properties of functionalized metallicity sorted single walled carbon nanotubes
- 20:00 **Poster II**

Tuesday, March 6th

Carbon nanotube spectroscopy

08:30**Probing Interactions in Single- and Few-Layer Graphene by Optical Spectroscopy**Tony F. Heinz¹¹Department of Physics, Columbia University, New York, NY 10514 USA

The optical conductivity of graphene provides a sensitive probe not only of the band structure, but also of various interactions in the system. We discuss three recent investigations.

(1) While the flat optical conductivity of graphene at low photon energies conforms to band structure calculations, at higher photon energies, we observe a strong deviation from this result. The existence of a peak around 4.5 eV can be understood within a single-particle picture. Its asymmetrical shape can, however, only be explained by excitonic (e-h) interactions.

(2) The interactions between different layers produces distinct low-energy band structure in few-layer graphene. We discuss the manifestations of band structure in the optical conductivity, emphasizing the role of stacking order (ABA or ABC) in few-layer graphene.

(3) The IR conductivity also permits probing of C-C stretching (G-mode) vibrations in few-layer graphene. We show the existence of strong coupling between these discrete modes and the electronic absorption continuum. The line shape of the modes is of a Fano form and varies significantly with layer thickness and stacking order.

09:00**Raman characterization of nanocarbons**Gustavo Cancado¹, Newton Barbosa¹, Jaqueline Soares¹, Rodolfo Maximiano¹, Ado Jorio¹¹Universidade Federal de Minas Gerais (UFMG), Belo Horizonte MG, Brazil

This talk presents an overview on the characterization of nanocarbons using Raman spectroscopy. The first part shows some developments of the technique applied to nanopgraphites and graphene. For nanographites, Raman spectroscopy delivers fast information about crystallite size and degree of stacking order. The Raman spectrum of graphene probes defect density, number of graphene layers, doping level, and the relative rotational angle of superlattices. In both cases, the Raman signal obtained from edges provides information about the atomic structure. We also extract the coherence length L of photo-excited electrons from the spatial confinement of the defect-induced Raman D band near the edges of graphene. Temperature dependent measurements in the range of 1.55K to 300K yield L proportional to $T^{-1/2}$. The second part of the talk shows theoretical and experimental results on the near-field Raman enhancement of 1D and 2D systems. The theory explains the dependency of the near-field Raman intensity on the tip-sample distance, and also on the geometrical parameters of the experiment (e.g. light polarization and tip-sample orientation).

09:30**Intrinsic optical properties of free-standing carbon nanotubes and graphene monolayers**

Stéphane Berciaud¹, Hootan Farhat², Rohit Narula^{2,3}, Xianglong Li⁴, Stephanie Reich³, Mildred S. Dresselhaus², Jing Kong², Stephen K. Doorn^{2,4}, Louis E. Brus⁵, Tony F. Heinz⁵

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²MIT, Boston, USA

³Freie Universität Berlin

⁴Los Alamos National Lab, USA

⁵Columbia University

The physical properties of carbon nanotubes and graphene are dramatically affected by the interaction between the substrate on which they are deposited. If, for practical purposes, substrate engineering is a valuable strategy, it is highly desirable to perform fundamental studies on pristine, free-standing samples.

We will present intrinsic features that have been observed in the inelastic light scattering spectra of free-standing, isolated, metallic single-walled carbon nanotubes (MSWNTs) and free-standing pristine graphene monolayers.

First, we will introduce electronic Raman scattering (ERS) in free-standing MSWNTs. The optical resonances in MSWNTs give rise to well-defined ERS peaks that are a unique feature of the electronic structure of MSWNTs.

Second, we will describe the intrinsic lineshape of the popular two-phonon intervalley Raman 2D mode in graphene monolayers. This feature consistently shows clear deviations from a Lorentzian form and broadens as the photon energy is decreased, i.e. as the momenta of the probed optical phonons approach the zone edge. In contrast, the neighboring supported regions exhibit a quasi-Lorentzian 2D mode feature.

10:30**Dominant phonon wavevectors and strain-induced splitting of the 2D Raman mode of graphene**Rohit Narula¹, Nicola Bonini², Nicola Marzari³, Stephanie Reich¹¹Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, Berlin 14195, Germany²Department of Physics, King's College London, Strand, London WC2R 2LS, United Kingdom³Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We use a combination of ab initio calculations and a full two-dimensional integration of the transition matrix to determine the dominant phonon wavevectors q^* probed by the 2D Raman mode of pristine and uniaxially tensile strained graphene. The q^* distribution is highly anisotropic and undergoes a rotation about K on sweeping the polarizer:analyzer orientation with respect to the lattice. The corresponding phonon-mediated electronic transitions show a finite component along $K - \Gamma$ that sensitively determines q^* , thus also highlighting the inadequacy of a one-dimensional treatment. We completely revoke the concept of 'inner' and 'outer' processes. We further demonstrate that the characteristic splitting of the 2D mode of graphene under uniaxial tensile strain and given polarizer:analyzer setting can only be reproduced faithfully once both the changes in the electronic bandstructure and the red-shift and strain-induced distortion of the iTO phonon dispersion are accounted for.

11:00**Theory of Raman spectroscopy of graphene on different substrates**Ludger Wirtz^{1,2}, Alejandro Molina^{1,2}, Adrien Allard², Florian Forster³, Christoph Stampfer³¹Laboratory for the Physics of Advanced Materials, University of Luxembourg, Luxembourg²Institute for Electronics, Microelectronics, and Nanotechnology (IEMN), CNRS, Lille, France³JARA-FIT and II. Institute of Physics B, RWTH Aachen University, Germany

We present ab-initio calculations of phonons of graphene on different metallic and non-metallic substrates. The changes in the phonon dispersion on metallic substrates can be quite pronounced depending on the degree of hybridization of the carbon π -bands with the surface states [1]. In particular, in the case of chemisorption on a Ni(111) surface, the Kohn-anomalies in the highest optical branch are suppressed and the strong Raman signal disappears. The changes on non-metallic substrates are more subtle. We compare the spectra of graphene on silicon dioxide with the spectra of suspended graphene [2] and graphene on hexagonal boron nitride [3]. We show that the screening by the substrate influences the electron-phonon coupling between the highest optical phonon branch at K and the π -bands. This mechanism is responsible for the shift of the Raman 2D line on different substrates.

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11:30**Double-resonant Raman modes in few-layer graphene**Janina Maultzsch¹¹Technische Universität Berlin, Berlin

The double-resonant Raman process in graphene and related materials allows determining the properties of electrons and phonons and their interaction throughout the Brillouin zone. Therefore it is important to understand the relevant double-resonance processes, in order to deduce which parts of the Brillouin zone contribute to the Raman modes. Here we show Raman experiments of suspended bilayer graphene combined with simulations, supporting the theoretical prediction that phonons with wave vectors between Gamma-K have the largest contribution to the 2D mode. Furthermore, we discuss double-resonant combination modes which can be used for alternative routes to determine the number of layers in few-layer graphene.

18:30**ESR from fully metal – semiconductor separated SWCNTs**

A. Chernov¹, M. Havlicek², W. Jantsch², Z. Wilamowski³, K. Yanagi⁴, H. Kataura⁵, M. H. Rummeli⁶, H. Malissa⁷, H. Kuzmany¹

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Electron spin resonance (ESR) from single-walled carbon nanotubes (SWCNTs) has been a subject of extensive research in the recent past. SWCNTs allow to study 1D spin physics. Results of the ESR measurements of highly metal–semiconductor (M–SC) separated SWCNTs will be presented in the talk. The ESR response of M and SC SWCNTs for temperatures T between 0.39 and 200 K is different for the two systems. For the M nanotubes the signal originates from defect spins but interaction with free electrons leads to a larger line width and decrease of the width with the increasing T . For SC nanotubes the line width increases with T .

For both systems the spins undergo a ferromagnetic phase transition around 10 K. Indirect exchange is suggested to be responsible for the spin-spin interaction, supported by RKKY interaction in the case of M tubes. For SC tubes spin-lattice relaxation via an Orbach process determines the line width.

M-SC separated SWCNTs have been filled with $FeCp_2$ and transformed to DWCNTs. Analysis was performed by ESR, Raman, TEM and XRD. In addition to DWCNTs the presence of ferromagnetic precipitates was detected.

Funding by FWF is acknowledged.

Tuesday, March 6th

Carbon nanotube spectroscopy

19:00

Ultrafast confocal microscopy and CT dynamics

Guglielmo Lanzani¹

¹iit-Politecnico di Milano, Milan

By using a confocal microscopy set-up pump-probe spectra and time traces can be obtained from sample area in the order of 0.5 micron. This unravel new dynamics, not detected with standard space averaging experiments. The talk will focus on the initial charge separation event following photo-excitation in photovoltaic blends. New experimental and theoretical evidences for the initial charge transfer state will be shown. Finally a new concept for energy harvesting by exploiting ordered nanodipoles in multi-stack nanostructures will be proposed.

19:30**Electronic transport properties of functionalized metallicity sorted single walled carbon nanotubes**Thomas Pichler¹¹Faculty of Physics, Vienna, Vienna

In this contribution I will present our recent progress on unraveling the influence of metallicity on the electronic transport properties of functionalized single walled carbon nanotubes. Photoemission and x-ray absorption spectroscopy were applied on fully metallicity sorted starting material to determine the bonding environment, influence of charge transfer, hybridisation and the influence of basic correlation effects on the two particle excitation and the nature of the metallic ground state as a function of metallicity and functionalisation. As examples a gas sensing model shows how reactive gases like nitrogen oxides are predominantly physisorbed with a weak chemisorption which depends on the metallicity of the SWCNT. The chemical reaction with the metallic SWCNT is stronger. Similar trends are observed regarding the charge transfer and hybridisation in metallicity sorted ferrocene filled SWCNT. Last but not least, the nature of the metallic ground state of filled as well as intercalated SWCNT was determined as function of the interaction of purely metallic and semiconducting SWCNT with the fillers and intercalant.

Work supported by FWF and the EU.

TUE 1**Fetal bovine serum proteins do not determine cell fate on graphene**Marie Kalbacova¹, Antonin Broz¹, Martin Kalbac²¹Institute of Inherited Metabolic Disorders, 1st Faculty of Medicine, Charles University, Prague²J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of CR, Prague, Czech Republic

The influence of single-layer graphene produced by chemical vapor deposition on human osteoblast cells under different conditions was studied. Measurements probed the ability of cells to adhere to and proliferate on graphene compared to SiO₂/Si substrates and standard tissue culture plastic when cells were incubated for the first 2 h in the presence or absence of fetal bovine serum (FBS), thus influencing the initial, direct interaction of cells with the substrate. It was found that after 48 h of human osteoblast incubation on graphene films there was a comparable number of cells of a similar size irrespective of the presence or absence of serum proteins. On the other hand, a strong, initial influence through the presence of FBS proteins on cell number and cell size was observed in the case of the SiO₂/Si substrate and control plastic. Thus, our study showed that the initial presence/absence of FBS in the medium does not determine cell fate in the case of a graphene substrate, which is very unusual and different from the behavior of cells on other materials.

TUE 2**Bolometric effects in the low temperature microwave absorption of single-wall carbon nanotube**Anita Karsa¹, Dario Quintavalle¹, László Forró², Ferenc Simon^{1,3}¹Department of Physics, Budapest University of Technology and Economics, Budapest²Laboratory of Physics of Complex Matter, FBS Swiss Federal Institute of Technology (EPFL), 1015 Lausanne, Switzerland³Universität Wien, Fakultät für Physik, Strudlhofgasse 4, 1090 Wien, Austria

We study the low temperature microwave absorption properties of single-wall carbon nanotubes using the microwave cavity perturbation method with a time resolved technique. The anomalous, non-linear microwave absorption (NLMWA) is observed around 20 K in agreement with previous studies [1]. The microwave absorption due to the sample follows the change in the microwave power with a slow, few second timescale dynamics. This rules out an electronic origin for the NLMWA in contrast to previous descriptions and rather points to a heating effect as its most probable origin. The connection between the NLMWA and other spectroscopic studies, which also indicate a low temperature anomaly, is discussed [2].

[1] B. Corzilius, K.-P. Dinse, J. van Slageren, and K. Hata, Phys. Rev. B 75, 235416 (2007).

[2] V. Likodimos, S. Glenis, N. Guskos, and C. L. Lin, Phys. Rev. B 76, 075420 (2007).

TUE 3**Electronic Properties of Single-Walled Carbon Nanotubes Intercalated by One-Dimensional Nanocrystals of Inorganic Chemical Compounds**

Marianna V. Kharlamova¹, Andrei A. Eliseev¹, Lada V. Yashina², Alexey V. Lukashin¹, Yury D. Tretyakov¹

¹Moscow State University, Department of Materials Science, Moscow

²Moscow State University, Chemistry Department, Moscow

Currently, the researchers are focused on finding tools to govern the electronic structure of nanostructures designed on the basis of single-walled carbon nanotubes (SWCNTs). One of the approaches is given by filling of internal channels of nanotubes with appropriate substances. In some cases, this approach makes it possible to get the material with well-defined electronic structure and properties even without separating of SWCNTs on their size and chirality. We performed the synthesis of 1D nanocrystals (GaX, SnX, Bi₂X₃, MHal_n, where X=S, Se, Te, M=Zn, Cd, Tb, Tm, Pr and Hal=Cl, Br, I) in channels of SWCNTs with inner diameter of 1-1.4 nm. The crystal structure of 1D nanocrystals was determined from HRTEM measurements and DFT calculations. According to XPS data and work function measurements, Fermi level downshift was observed for SWCNTs intercalated by metal halides. At the same time, XPS and Raman spectroscopy data for SWCNTs filled with Sn and Bi chalcogenides indicated that there were no noticeable interactions between the 1D crystals and nanotubes. Based on a whole dataset, a self-consistent picture of the nanocrystal-SWCNT interactions was derived.

TUE 4**Reductive Multiple Addition on Graphene**

Kathrin C. Knirsch¹, Jan M. Englert¹, Frank Hauke¹, Andreas Hirsch¹

¹University of Erlangen-Nuernberg, Institute of Advanced Materials and Processes, Dr.-Mackstr. 81, Fuerth, Germany

From a chemist's point of view, a fundamental aim of carbon allotrope research is and has been -the covalent functionalization of the carbon framework-, enabling the modification of the materials' surface properties, which leads to tailored characteristics for numerous applications. The functionalization in general boosts the solubility of the novel nanomaterial graphene, modifies the outstanding characteristic electronic and physical properties and allows the combination with other compounds, e.g. porphyrins. Recently, the covalent functionalization of graphene has already turned out to be successful in terms of a wet chemical bulk-functionalization reaction. The main focus of this work is based on iterative multiple functionalization sequences of three different types of graphite as starting material. The detailed analysis by statistical Raman spectroscopy revealed the pronounced impact of the starting material with respect to the degree of functionalization. In analogy to fullerene and carbon nanotube chemistry, a retrofunctionalization could also be proven

for the first time. The mixed functional adducts furthermore reveal the outstanding possibilities of graphite chemistry.

TUE 5

Theory of time- and momentum-resolved carrier dynamics in CNTs

Christopher Köhler¹, Tobias Watermann², Olga A. Dyatlova¹, Ulrike Woggon¹, Andreas Knorr¹, Ermin Malic¹

¹Institut für Theoretische Physik, TU Berlin, Berlin

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We investigate the time- and momentum-resolved relaxation dynamics of non-equilibrium charge carriers driven by optical and acoustic phonons in semiconducting carbon nanotubes. Within the density matrix formalism, we derive microscopic Boltzmann-like equations describing scattering processes via carrier-phonon channels. We obtain an ultrafast relaxation on the femtosecond timescale, which we ascribe to the scattering with optical phonons [1]. In contrast, the acoustic phonons lead to a relaxation on the picosecond timescale due to the weaker coupling elements. Our results are in good agreement with recent experiments [2]. Furthermore, we study carrier relaxation dynamics for a variety of nanotubes with different diameters and chiral angles as well as for different excitation energies. We find the fastest dynamics for zig-zag tubes with a small diameter.

[1] C.Köhler, T. Watermann, A. Knorr, and E.Malic
Physical Review B **84** 153407 (2011).

[2] O.A. Dyatlova, C. Köhler, E.Malic, J. Gomis-Bresco, J. Maultzsch, A. Tsagan-Mandzhiev, T. Watermann, A. Knorr, and U. Woggon
submitted for publication (2011).

TUE 6

Electron and ion irradiation effects on graphene from theory and experiments

Jani Kotakoski^{1,2,3}, Simon Kurasch², Ossi Lehtinen^{2,3}, Harriet Åhlgren³, Franz Eder¹, Viera Skákalová^{1,4}, Jurgen H. Smet⁴, Ute Kaiser², Arkady V. Krasheninnikov^{3,5}, Jannik C. Meyer¹

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⁴MPI Stuttgart, Germany

⁵Aalto University, Finland

High resolution transmission electron microscopy (HRTEM) has allowed the imaging of atomic-scale defects in graphene [1] and other materials. At the same time interesting atomic-scale processes – induced by the imaging electrons while they traverse the sample – have been revealed. We have studied these effects combining HRTEM and density-functional theory-based computer simulations and demonstrated, .e.g, amorphization of graphane [2], bond-rotation-driven migration of defects [3], edge transformations [4] and shrinkage of small grains until disappearance. Graphene also serves as the perfect membrane for ion irradiation of volatile samples. However, the usability of such a membrane depends heavily on its irradiation response. At the same time ion beams can be used to dope and/or cut this material. All of these issues can be studied applying atomistic simulations [5-7], as will be described in the second part of this presentation.

- [1] ACS Nano 5, 26-41 (2011)
- [2] Phys. Rev. Lett. 106, 105505 (2011)
- [3] Phys. Rev. B 83, 245420 (2011)
- [4] ACS Nano, doi: 10.1021/nn204148h
- [5] Phys. Rev. B 81, 153401 (2010)
- [6] Nanotech. 22, 175306 (2011)
- [7] Phys. Rev. B 83, 115424 (2011)

TUE 7

Diameter specific growth of sub-nm thin SWCNT

Christian Kramberger¹, Theerapol Thurakitseree¹, Shiego Maruyama¹

¹Department of Mechanical Engineering, University of Tokyo, Tokyo

The bulk scale separation of SWNT is a major breakthrough in nanotechnology. Concerns on achievable purity and efficiency stimulate ever more demand for the enriched growth of specific chiralities.

Conventional wisdom dictates that the diameter control in the CVD growth of SWCNT requires in some way control of the catalyst morphology. The use of acetonitrile/ethanol mixed feedstocks is a noteworthy exception to that rule.

We quantitatively correlate drastically reduced mean diameters with the incorporation of substitutional sp² nitrogen [1]. Growth stemming from the pores of zeolite yields very narrow diameters. Still, the mean diameter as well as the distribution width are significantly further reduced upon adding acetonitrile to the ethanol feedstock. Combined Raman and PLE mapping evidence on the bulk scale specific enrichment for the abundance of individual chiralities.

- [1] T. Thurakitseree et al. Carbon, submitted

TUE 8**CNT growth utilizing C:Ni nanocomposites**

Matthias Krause^{1,2}, Miro Haluska³, Robert Wenisch², Gintautas Abrasonis², Sibylle Gemming²

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Precise control of single walled carbon nanotube (SWCNT) diameter, chirality, alignment, and intertube arrangement are still remaining challenges in the catalytic chemical vapour deposition (CCVD) synthesis. In this context it has to be clarified whether a predefined size and shape of the nanoparticles can be stabilized by a suitable matrix material while preserving the catalytic activity of the particle. For this study Ni nanoparticles were encapsulated in an amorphous carbon matrix by physical vapour deposition. As prepared Ni catalysts were used for CNT fabrication by laser assisted CVD applying either no external carbon source or C₂H₄ gas, and by low pressure CVD applying C₂H₂ or CH₄ as carbon source. The broad range of CNT synthesis conditions indicates the robustness of the embedded Ni particles as a catalyst for carbon nanotube formation. SEM and laser wavelength dependent Raman spectroscopy were used for CNT characterisation. The nickel-SWCNT-interaction was modelled by density functional calculations with the projector augmented plane wave method, utilizing the generalized gradient approximation for the exchange-correlation functional.

TUE 9**150-GHz Carbon Nanotube Array Field-Effect Transistors**

Mathias Steiner¹, Michael Engel^{2,3}, Yu-Ming Lin¹, Yanqing Wu¹, Keith Jenkins¹, Damon B. Farmer¹, Nathan Yoder⁴, Ted J. Seo⁵, Alexander A. Green⁵, Mark C. Hersam⁵, Ralph Krupke^{2,3,6}, Phaedon Avouris¹

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Carbon nanotubes (CNT) are a promising candidate for high-frequency, possibly THz, electronic applications due to their high saturation carrier velocity. We produced CNT array field-effect transistors based on centrifugation-enriched solu-

tions containing 99.6% semi-conducting CNTs. A novel CMOS-compatible planar device platform with embedded electrodes allows for the controlled, independent scaling of channel length, gate length, gate dielectric thickness, and contact length. Furthermore, it allows for situ ac-field driven dielectrophoresis assembly of aligned dense CNT arrays. We carried out DC and high-frequency characterization of as fabricated CNT devices. The DC output characteristics show clear current saturation important for power amplification. For high-frequency characterization we performed standard S-parameter measurements in order to extract cut-off frequencies and maximum frequencies of oscillation. We achieved a record intrinsic cut-off frequency of 150GHz and power gain up to 30GHz. The semi-conducting nature of our CNTs suggests higher gain and lower power dissipation compared to the similar material of graphene.

TUE 10

High-pressure infrared transmission studies on SWCNTs, C₆₀ Peapods, and DWCNTs

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The shape of single-walled carbon nanotubes (SWCNTs) is deformed from circular to oval at a critical pressure $P_c = 2-3$ GPa. Further increase in the applied pressure deforms the shape to a more flat structure at a pressure of 5-6 GPa [1]. The stabilization of SWCNTs against collapse by filling the empty tubes with fullerene molecules or with an inner tube is an important issue. Recently, high-pressure Raman measurements showed that in the case of double-walled carbon nanotubes (DWCNTs) the inner tube supports the outer one up to high pressure before the collapse. On the contrary, C₇₀ peapods collapse at lower pressure values compared to the empty SWCNTs [2]. To elucidate this issue, we carried out high-pressure infrared transmission studies on SWCNTs, C₆₀ peapods, and DWCNTs up to 20 GPa using alcohol mixture as pressure transmitting medium. Our results show that both fillers greatly influence the pressure-induced effects in SWCNTs. They will be compared to those in Ref. [2].

[1] C. A. Kuntscher et al., Phys. Stat. Sol. (b) **247**, 2789 (2010). [2] A. L. Aguiar et al., J. Phys. Chem. C **115**, 5378 (2011).

TUE 11

Annealing of small grains in graphene under low-energy electron irradiation

Simon Kurasch¹, Jani Kotakoski^{2,6}, Ossi Lehtinen², Carl E. Krill III³, Viera Skákalová^{4,6}, Jurgen H. Smet⁴, Arkady V. Krashenninnikov⁵, Ute Kaiser¹

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Irradiation is typically considered to be detrimental to any material. Indeed, extensive studies performed on graphene have demonstrated that electron irradiation can cause sputtering [1] or other structural changes [2] in this atomically thin two-dimensional carbon membrane, depending on the acceleration voltage. But electron irradiation can have a positive influence on the structure of graphene, as well. Here, by combining low-energy (80 kV) aberration-corrected high-resolution transmission electron microscopy of graphene with density functional theory calculations and Metropolis Monte Carlo modeling, we show that the non-ideal configurations of grain boundaries in as-grown polycrystalline graphene can be modified under electron irradiation. In fact, small grain domains (1–2 nm) can be completely healed out in this manner.

Our results give new insight into the atomic structure of graphene grain boundaries and small grains, as well as into their dynamics, and could pave the way toward the development of new methods for engineering the microstructure of nanomaterials.

[1] C. O. Girit et al., *Science* 323, 1705 (2009)

[2] J. Kotakoski et al., *PRL* 106, 105505 (2011)

TUE 12

Carbon nanobamboo: junctions between left and right handed single walled nanotubes

Jenő Kürti¹, János Koltai¹, Viktor Zólyomi², Ádám Rusznyák¹, Zoltán Kruppa¹

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Heating of organic molecules, e.g. fullerenes encapsulated in single walled carbon nanotubes can result in coalescence of the molecules forming an inner tube. Growth of tubes with different diameters and/or chiralities can start at different places at the same time. The formation of a junction between the two different tubes depends on many parameters. A special case is when the two tubes have the same chiralities, but opposite handedness. We have shown using topological arguments that at least two non-equivalent junctions can be formed in these cases, with different arrangement of the pentagons and heptagons in the junction. We optimized the geometry using DFT method and investigated the effect of the junction on the electronic density of states of the bamboo-type nanotube.

TUE 13**Ferromagnetic decoration in metal-semiconductor separated and ferrocene functionalized single-walled carbon nanotubes**

Hans Kuzmany¹, A. Chernov¹, H. Peterlik¹, M. Havlicek², W. Jantsch², M. H. Rummeli³, A. Bachmatiuk³, K. Yanagi⁴, H. Kataura⁵, F. Sauerzopf⁶, R. Resel⁷, F. Simon⁸

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⁷Technische Universität Graz, Graz, A

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We report structural and magnetic analyses of fully metal (M)-semiconductor (SC) separated SWCNTs prepared from non magnetic catalyst PtRhRe and functionalized by ferrocene (FeCp₂). TEM analysis revealed almost full removal of amorphous carbon and catalyst particles by the purification and separation process. However, even for the purified samples substantial features remain on the surface of the tubes, suggested to originate from amorphous carbon and surfactants. After functionalizing the tubes with FeCp₂ ESR and SQUID measurements revealed ferromagnetic contributions. In the M tubes they clearly originate from magnetite (Fe₃O₄) and undergo a well known Verwey transition at 100 K. The presence of magnetite is confirmed from x-ray analysis. SC tubes also exhibit a Verwey-like transition but magnetic grains are much smaller and extend into the nm range. Also, additional magnetic phases are observed. The growth of these phases is suggested to originate from a reaction of FeCp₂ with oxygen from the surfactants on the surface of the tubes forming a magnetic decoration.

Supported by the FWF, Projects P20550 and P21333-N20

TUE 14**in situ and ex situ time resolved study of multi-component Fe-Co oxide catalyst activation and carbon deposit nucleation during MWNTs synthesis**

Vladimir L. Kuznetsov^{1,2}, Dmitriy V. Krasnikov², Alexander N. Schmakov^{1,2}, Karina V. Elumeeva¹, Sergey N. Trukhan¹, Stanislav S. Yakushkin¹, Oleg N. Martynov¹, Aleksander V. Kalinkin¹, Igor P. Prosvirin¹

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The number of CNTs potential applications has grown enormously ranging from nanoelectronic to multifunctional composite materials. The effectiveness of these

applications depends on properties of individual tubes. CNT properties are altered by diameter distribution, morphology, defectiveness and number of layers in each individual CNT, which are in turn depend on CNTs' growth conditions and catalyst properties. It was found that multi-component Fe-Co oxide catalysts have benefit in comparison with mono-component catalysts because of their higher activity. Due to of key role of catalysts in production of specific types of CNTs we have performed study of catalyst activation and CNT nucleation using in-situ X-ray diffraction on synchrotron radiation, in-situ X-ray photoelectron spectroscopy, in-situ ferromagnetic resonance combined with ex situ HR TEM study and kinetic studies of CNT formation provided time resolved information on the subject of structural and chemical states of species involved in catalytic reaction. Obtained results can be used for optimization of in-situ catalysts activation in catalytic CVD process for production of MWNTs with predetermined properties.

TUE 15

Molecular dynamics simulation of carbon nanostructures

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Molecular dynamics calculations can reveal the physical and chemical properties of various carbon nanostructures or can help to devise the possible formation pathways. In our days the most well known carbon nanostructures are the fullerenes and the nanotubes. They can be thought of as being formed from graphene sheets, i.e. single layers of carbon atoms arranged in a honeycomb lattice. Usually the nature does not follow the mathematical constructions. An ideal nanotube can be thought of as a hexagonal network of carbon atoms that has been rolled up to make a cylinder. There is not any theory of carbon nanotube formation which is based on this construction. Although the first time the C₆₀ and C₇₀ were constructed by laser irradiated graphite, the fullerene formation theories are based on various fragments of carbon chains, and networks of pentagonal and hexagonal rings. In the present talk various formation pathways for carbon nanostructure formations will be studied in the frame work of molecular dynamics calculations. Suggestions will be given for practical experimental realizations.

TUE 16

Resonance behavior of the defect-induced Raman mode in metallic and semiconducting carbon nanotubes

Jan Laudénbach¹, Ninette Stürzl², Frank Hennrich², Manfred Kappes², Edib Dobardžić³, Ivanka Milosević³, Milan Damnjanović³, Janina Maultzsch¹

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³Faculty of Physics, University of Belgrade, Belgrade, Serbia

Functionalization of single-walled carbon nanotubes (SWCNTs) leads to an increase in intensity of the defect induced Raman bands. A large intensity of the defect modes is therefore often used as an evidence for successful functionalization. However, there is no hint if a selective functionalization of metallic or semiconducting SWCNTs can be confirmed with the help of the intensity or position of the defect mode. A necessary condition would be that the resonance profiles of the defect modes are known in comparison to the profiles of the well-known radial-breathing modes. Here we analyze the Raman defect modes of (9,7) enriched semiconducting SWCNT samples [1]. By resonance Raman spectroscopy we study the intensity of the defect mode of SWCNTs for excitation energies in the range of 1.49 - 2.05 eV. Furthermore, we compare our experimental results with numerical simulations of the Raman spectra and calculation of the resonance behavior of the defect mode. We show that near resonance the defect mode is strong enhanced and the dispersion differs from the well-known linear behavior away from resonance.

[1] Stürzl et. al JACS 2009, 113, 14628-14632

TUE 17

Spin Arrangements in Quasi One-dimensional Systems

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Geometrical symmetries of regular quasi-one-dimensional (Q1D) systems, including various types of nanotubes or polymers, are gathered into line groups [1]. Magnetic properties of materials are determined by spin arrangements. Their symmetry involves time reversal in addition to the geometrical transformations. In this sense, spin arrangement in a Q1D system must be invariant under either line group $L = L' + l^*L'$ or one of the associated black-and-white groups $M(L) = L' + \theta l^*L'$ (L' is a halving subgroup of L and l^* is any of the remaining elements). We propose an algorithm to get allowed invariant spin orientations for all the orbits of the line groups. It can be generalized to arbitrary (multiorbit) systems, i.e. systems with chemically different species. This way we single out possible ferromagnetic, anti-ferromagnetic and very interesting helix-like spin arrangements of Q1D systems. Possible spin-waves theories based on various dynamical models and applications are discussed.

[1] M. Damnjanovic, I. Milosevic, Line Groups in Physics, Lecture Notes in Physics 801 (Springer, Berlin-Heidelberg, 2010)

TUE 18**Molecular Beam Epitaxy of Graphene on Mica**

Gunther Lippert¹, Jarek Dabrowski¹, Yuji Yamamoto¹, Felix Herziger², Janina Maultzsch², Jens Baringhaus³, Christoph Tegenkamp³, Max C. Lemme⁴, Grzegorz Lupina¹

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Graphene device fabrication in silicon mainstream technology is limited in temperature budget and low density of defects and impurities in the process.

To meet these requirements – the growth of graphene on inert model substrate (Al-silicate – mica) by molecular beam epitaxy (MBE) at growth temperature below 1000°C has been investigated. UHV-sublimation of carbon onto the mica surface results in the formation of single-, bi-, and multilayer graphene layers with the size in the micrometer regime. According to the Raman D mode, the grown graphene shows no remarkable defects. The Raman spectra are analysed in detail and compared with the spectra of a single layer of exfoliated graphene. The shape of the 2D mode indicates the presence of single-layer graphene in the MBE-grown sample. The ratio of the mode 2D/G and the defect density are similar between grown and exfoliated single layer graphene on mica. Local four-point probe transport measurements in STM show, the low sheet resistance (500 Ohm/sq) measured at room temperature depends not on the probe spacing as expected for a 2d electron gas. Density functional theory calculations support the understanding of the growth mode.

TUE 19**The Crystal Structure and Raman Spectra of $\text{closo-}[\text{Ge}_9]^{2-}$, $\text{polymeric-}[\text{Ge}_9]^{2-}$, and $\text{nido-}[\text{Ge}_9]^{4-}$ Zintl anion clusters**

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¹Texas Center for Superconductivity, University of Houston, Houston

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Single crystals of $[\text{K}([2.2.2]\text{crypt})]_2\text{Ge}_9$ (**1**), $(\text{K}[18\text{-crown-6}])_2\text{Ge}_9\text{-en}$ (**2**) and $\text{Cs}_4\text{Ge}_9\text{-en}$ (**3**) were prepared by the reaction of alkali metal-germanium alloys, with [2.2.2] cryptand, 18-crown-6 in ethylenediamine and toluene. The crystal structures were refined from single crystal X-ray diffraction features of isolated nine-atom Ge_9^{n-} ($n=2,4$) anions in compounds **1** and **3** and a polymeric chain of Ge_9^{2-} clusters in

2. The crystal structures also feature the corresponding complex and monoatomic cations, and solvent molecules. However, unambiguous determination of the cluster symmetry can not be performed for the Ge_9^{2-} anions in **1** due to severe crystallographic disorder. Polarized Raman scattering experiments on different single crystals of all three cluster compounds were carried out at room temperature. Analysis of the experimental vibrational spectra and comparison with the results of the density functional theory calculations allowed us to confirm D_{3h} , C_{2v} , and C_{4v} point symmetries for the cluster anions Ge_9^{2-} , polymeric Ge_9^{2-} , and Ge_9^{4-} , respectively.

TUE 20

Evidencing the correlation between catalyst particles and single-wall carbon nanotubes : a first step towards chirality control

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Controlling the SWNT structure in CVD remains an hot challenge. Here, by studying in a systematic way, using ex situ TEM, the structure of the tubes and the particles from which they grow and of their link, we inspect how the SWNT diameter is driven by the particle. We used a specific synthesis protocol, making possible the direct observation of both the tubes and their seed particles at any stage of the growth and performed a statistical study of the nano-objects at different synthesis times. At the early stages, two nucleation modes are identified, depending on whether the tube nucleates tangentially or perpendicularly to the surface of the nanoparticle, whatever its size. Then, only nuclei tangentially linked to particles with defined diameter give rise to long tubes. Tight-binding calculations have been performed to understand the origin of the nucleation mode selectivity. The tangential mode is found to be the most stable one, suggesting that the perpendicular mode is driven by kinetics effects, and that steady state conditions with low growth rates should be looked for favoring the tangential mode and achieving a direct control of the nanotube diameter by the particle size.

TUE 21

Hydrogenation, purification and unzipping of carbon nanotubes by reaction with molecular hydrogen: road to graphane nanoribbons

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Reaction of single-walled carbon nanotubes (SWNTs) with molecular hydrogen was studied at hydrogen pressure of 50 bar and temperature interval of 400-550°C. Side wall hydrogenation of nanotubes was observed at 400-450°C with up to 1/4 of carbon atoms forming C-H bonds. The hydrogenation becomes possible due to catalytic effect of Fe nanoparticles which dissociate molecular hydrogen to atomic with subsequent reaction of atomic hydrogen with nanotubes. At higher temperatures (500- 550°C) hydrogen reaction with SWNTs occurs with etching and formation of light hydrocarbons. Hydrogenation was shown to be an efficient tool for SWCNTs opening and purification from other forms of carbon as well as for removal of fullerene-like cups covering metal particles. Prolonged hydrogenation resulted also in partial SWNTs unzipping and formation of graphene nanoribbons. Products of SWNTs hydrogenation were studied with IR and Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), near-edge X-ray adsorption fine structure (NEXAFS), and transmission electron microscopy (TEM).

TUE 22

Growth of Graphene by Chemical Vapour Deposition (CVD) using Oxidative De-Hydrogenation Chemistry

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Application of graphene is foreseen in composites, energy production and storage devices, touch screens and electronics. This conviction is the result of theoretical predictions of graphene properties, and relies on the outstanding performances of small sized prototypes fabricated with graphene exfoliated from graphite. Most predictions are yet to be verified experimentally while specifications of large-scale devices remain uncertified. To meet these objectives, extended films of high-quality graphene need to be produced reliably.

CVD is the most suitable process yielding graphene from hydrocarbons over transition metal substrates. The most efficient synthesis proceeds from methane at elevated temperature and is not compatible with most applications.

The use of oxidative dehydrogenation (ODH) is very promising for graphene by CVD as such chemistry has allowed the growth of carbon nanotubes with low defect density down to 300°C. [1] We will report on the optimisation of the ODH parameters shedding light on graphene growth mechanism. Transport and optical

properties of graphene by ODH will be compared with graphene from methane.

1. Magrez et al, ACS Nano 2011

TUE 23

Self-organized fluorine chains on graphene planes

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Second-stage inclusion C₂F compounds represent the system of loosely bonded semifluorinated bilayer graphenes. Using the method of room-temperature wet fluorination, we obtained planar fluorinated graphene sheets where the contribution of magnetism from isolated defects and from the edge spins is minimized giving the possibility to study the basal plane inherited carbon magnetism. The mechanism of fluorination assumes the random attachment of primary fluorine atom to graphite network and further random direction of chain formation. When the process of wet synthesis is finished, the fluorine atoms continue reorganizing on the basal plane: isolated fluorine atoms diffuse rapidly along a path above C-C bonds till the structure reaches the energetically preferable state. A joint experimental and theoretical investigation suggests a description of this compound as coupled alternating antiferromagnetic Heisenberg chains. Magnetization measurements evidence a spin gap of about 110 K. Having performed the measurements on the same samples during 5 years, we followed the formation of bulk antiferromagnetic carbon in a self-assembly process.

TUE 24

Alumina chip cooling with integrated carbon nanotube microfin cooler

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Thermal properties of aligned carbon nanotubes (CNTs) together with the possibility of wafer-level integration with chips makes them promising candidates for implementing novel cooler structures with high performance. In this study, vertically aligned chemical vapor deposition (CCVD) grown multi-walled carbon nanotubes (MWCNTs) are used as an integrated microfin cooler on alumina chip. Test chips are fabricated on alumina template by thick-film technology and CNTs are transferred on chips by soldering with lead-free solder paste (Sn/Ag/Cu). CNTs are enhanced by a metal coating (Cr/Au, 15 nm/450 nm) to improve their solde-

ring properties and adhesion between CNTs and a metal electrode. Laser is used for structuring the micro-finned cooler structure. The cooling performance of the CNT-based cooler is tested and the results are compared to a reference cooler made from copper (Cu) having similar cooler geometry. The experimental results show good heat removal capability. The measurement results of the CNT cooler are comparable with the Cu reference cooler results. Possible improvements for enhancing the cooler performance in the future are also discussed.

TUE 25

Electron Transfer of non-covalent functionalized Graphene

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Graphene's extraordinary electronic properties render it a promising material for electronics, materials sciences, and photo conversion systems. We focus on integrating graphene into electron donor / acceptor hybrids by concomitant exfoliation of "natural graphite" as starting material. In this regard, we immobilized molecular building blocks, which are predestinated for $\pi - \pi$ stacking, as exfoliation reagents, e.g. porphyrins, phthalocyanines¹ or pyrene derivatives², onto graphene. In addition, the aforementioned building blocks are prone to react as either an electron acceptor or electron donor. A myriad of covalent or non-covalent means are at our disposal to combine graphene with appropriate functionalities resulting in complex electron donor-acceptor conjugates or hybrids for e.g. solar energy conversion, respectively. The energy and electron transfer interactions within these newly formed donor/acceptor nanohybrids are examined in depth by time-resolved and steady-state techniques.

[1] J. Malig et al, Angew. Chem. Int. Ed. 2011, 50, 3561.

[2] J. Malig, C. R. Nieto, N. Jux and D. M. Guldi, Adv. Mater. 10.1002/adma.201103697.

TUE 26

The effect of shock wave compression on double walled carbon nanotubes

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Recent experiments in a diamond anvil cell (DAC) [1,2] demonstrate high structural stability of double walled carbon nanotubes (DWNTs) exposed to a static pressure of 35 GPa. Here we report on the study of DWNTs after application of shock wave (dynamic) compression in a recovery assembly. In the different shock wave experiments the pressure was ramped to a certain level (14, 19, 26 and 36 GPa) with a new CNT sample but always from the same source batch. The recovered samples were characterized by Raman, XPS and HRTEM revealing outer wall disruption along with unzipping and shortening of the CNTs. Structural damage of the CNTs increases with the shock pressure. Simultaneously, the Raman data exhibit a steep increase of D/G-band intensity ratio. Remarkably, there are indications that the largest diameter CNTs were destroyed (RBM signal disappeared) by application of the highest shock contrary to the behavior of DWNTs at comparable static pressures. Along with the nature of the applied pressure, we discuss other possible reasons which may have caused such an effect.

[1] S. You, et al. High Pres. Res. 31, 186, 2011

[2] A.L. Aguiar, et al. J. Phys. Chem. C, 115, 5378, 2011

TUE 27

Magnetic Mott–Jahn–Teller ground states in expanded trivalent fullerides revealed by vibrational spectroscopy

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Strong electronic correlations play an important role in fulleride superconductors contrary to the widespread BCS scenario. Trivalent fulleride salts with an expanded lattice are Mott insulators which become metals on decreasing the lattice constant, and superconductors upon cooling from the metallic state. As the "Mottness" of these materials is confirmed by various magnetic measurements, here we reveal the other part, their "Jahn–Teller-ness". We do this by employing vibrational spectroscopy, which can detect even small molecular deformations that lower the symmetry. From temperature dependent infrared measurements we show evidence for a dynamic Jahn–Teller effect in expanded Cs-containing fullerides.

TUE 28**A New Complementary Vertical Graphene Transistor: Concept and Simulations**

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IHP is a research institute of Leibniz Association and has long term experiences in the field of RF devices and circuits. We have demonstrated SiGe:C HBTs with $f_{\text{max}}=0.5\text{THz}$ (IEDM 2011). To increase the frequency we have developed a new vertical graphene transistor concept. The graphene layer is used as an electrode that controls a hot carrier current from the emitter electrode to the collector. This new transistor concept has several advantages over the well-known graphene FETs. In particular, these new devices have a high $I_{\text{on}}/I_{\text{off}}$ ratio, natural current saturation, and are useable for analog radio frequency applications and as complementary transistors for ultra-high speed logic applications and also as high power transistors with collector voltages of more than 10 V. Conservative simulations have shown that cutoff frequencies up to 2 THz can be achieved.

TUE 29**Resonant Raman analysis of modified diamondoids**

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Diamantane functionalized with thiol, alcohol and amino groups [1,2] has been analysed by Raman spectroscopy. The spectra were assigned by supporting DFT computations, using the B3LYP functional and the basis set 6-311G(d) as implemented in the program Gaussian 09. Signatures of successful functionalization in the Raman spectra are discussed. Three fingerprint regions for a fast determination of successful functionalization are presented. With the help of these fingerprint regions we can distinguish between two different sites of the functional group. Further we analysed diamondoid compounds containing sp^2 -hybridized C-atoms. We observe strong enhancement of the double-CC-stretching mode at around 1700 cm^{-1} due to resonance in the deep UV region, indicating a modification of the electronic structure of the diamondoids due to the sp^2 -impurities.

[1] H. Schwertfeger, A. A. Fokin, and P. R. Schreiner, *Angew. Chem. Int. Ed.* 2008, 47, 1022/1036. DOI: 10.1002/anie.200701684

[2] B. A. Tkachenko, N. A. Fokina, L. V. Chernish, J. E. P. Dahl, S. G. Liu, R. M. K. Carlson, A. A. Fokin and P. R. Schreiner, *Org. Lett.* 2006, 8, 1767-1770

TUE 30**Carbon nanowalls synthesis by means of atmospheric dcPECVD method for supercapacitor applications**

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Graphene nanowalls have been considered to be a strong candidate for next generation electrode materials in supercapacitors. It is because of their unique physical properties, excellent chemical stability and exceptional large specific surface area. Carbon nanowalls (CNWs) are mainly synthesized by low -pressure hot filament CVD, radio frequency (rf) and microwave PECVD methods. Another approach for producing them is atmospheric dcPECVD method. This method allows CNWs to be synthesized in high rate due to the presence of larger amount of radicals. Furthermore this method is easier scaleable compare to the rf or microwave PECVD methods. CNWs were grown on Ni substrates at temperature of 800C in plasma environment of argon and hydrogen gas mixture flowing through the bubbler with ethanol and water. CNWs morphology investigations performed by scanning electron microscopy revealed that deposits consist of individual vertically oriented freestanding flakes. Role of the water on CNWs growth together with investigation of their structural properties will be discussed in detail.

TUE 31**Functionalization of carbon nanotubes with {Mn}-4 polymetallic complexes**

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Carbon nanotubes (CNTs) can be chemically modified in many ways by attaching molecules to the outside wall, to the tube ends or inside the inner hollow. Such functionalization of CNT transport devices leads to new applications, e.g., as chemical sensors or detectors. It can be achieved either by vanderWaals interactions or, in a more controlled way, by formation of covalent bonds. Here, we present covalent functionalization of CNTs with magnetic {Mn}-4 complexes. The route for this functionalization is very general, based on ligand exchange and can be applied for different types of molecules. The yield of the functionalization depends on the number of carboxylic groups on the CNTs created by oxidation. This process is monitored using Raman spectroscopy. However, the specific atomic structure can only be investigated by transmission electron microscopy (TEM). Scanning TEM

including elemental analysis by EDX and EELS reveals the functionalization on a molecular level. Finally, the changes in the magnetization behavior of the $\{\text{Mn}\}_4$ complexes bonded to the CNTs are analyzed using data obtained in temperature dependent SQUID measurements.

TUE 32

Rigid-plane phonon modes in layered crystals

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The lattice dynamics of low-frequency rigid-plane modes in metallic (graphene multilayers, GML) and in insulating (hexagonal boron-nitride multilayers, BNML) layered crystals is investigated by theory. The frequencies of shearing and compression (stretching) modes depend on the layer number N and are presented in the form of fan diagrams. The results for GML and BNML are very similar. In both cases only the interactions (van der Waals and Coulomb) between nearest-neighbor planes are effective, while the interactions between more distant planes are screened. A comparison with recent Raman scattering results on low-frequency shear modes in GML is made. Relations with the low-lying rigid plane phonon dispersions in the bulk materials are established. Master curves which connect the fan diagram frequencies for any given N are derived. Static and dynamic thermal correlation functions for rigid-layer shear and compression modes are calculated. The results might be of use for the interpretation of friction force experiments in multilayer crystals.

TUE 33

Stability and Mechanics of Carbon Nanocoils

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By means of the topological coordinate method and molecular mechanics based on the Brenner potential, structural model of the carbon nanocoils is proposed. Its stability is confirmed by the line group symmetry based density functional tight binding numerical calculations.

As due to their extraordinary elasticity carbon nanocoils are promising candidates for variety of the applications their stiffness, strength and super-elastic behavior are studied in detail.

TUE 34**Magnetic properties of $\text{Gd}_3\text{N@C}_{80}$**

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The long spin-lattice relaxation times and large magnetic moments of MRI contrast agents significantly increase the spin relaxation rate of water protons. Endohedral magnetic metallofullerenes, like water soluble $\text{Gd}_3\text{N@C}_{80}[\text{DiPEG}(\text{OH})_x]$, are ideal candidates for diagnostic biomedical nanoprobe. Here we investigate by high-frequency electron spin resonance (ESR) and SQUID magnetometry two key questions: How are the three magnetic Gd ions coupled to one another and what is the motional state of the $\text{Gd}_3\text{N@C}_{80}$ endohedral fullerene? SQUID magnetometry reveals that Gd^{3+} ions are ferromagnetically coupled at low temperatures and are uncoupled at high temperatures. The 210 and 315 GHz ESR measures at low temperatures magnetic excitations between the lowest Zeeman levels. At 2 K the 4 T broad ESR is well described by a single transition in static molecules broadened by fine structure effects. At higher temperatures there is a gradual transition between the static and rotating states. At ambient temperatures the rotation frequency is much larger than the fine structure broadening and a single ESR line is observed at $g=1.99$.

TUE 35**Strategies to link photosynthetic reaction centers to carbon nanotubes for efficient light energy conversion**

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Special interest is paid recently to bind photosynthetic reaction centers (RC) to nano structures, also to carbon nanotubes (NT). One reason is that RC is nature's

solar battery converting light energy into chemical potential very efficiently, so that any use in artificial systems would be profitable. The other reason is that being membrane protein, RC requires special environment for proper function. In order to explore the optimal conditions for the function of RC/NT bio-nanocomposite, RCs purified from *Rhodobacter sphaeroides* R-26 purple bacterium were bound to single- (SWNT) and multi- (MWNT) walled NTs through physical and specific chemical binding. Structural (EM, AFM) and kinetic (kinetic absorption change) measurements indicate that RC was functionally bound to the NT surface in both cases. It appears that physical binding between RCs and NTs provides better conditions for the photoelectric energy conversion in this hybrid nanosystem than chemical immobilization.

TUE 36

Chemical Vapor Deposition of Graphene: Growth, Transfer and Characterization

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Our goal is to investigate several properties of graphene and in particular electrical transport through constrictions and narrow gaps. To achieve this, we built a setup for chemical vapor deposition (CVD) growth of graphene on Cu foil, based on the process established by Ruoff et al. [1]. To fabricate high quality devices, a clean and crackless transfer of the graphene onto arbitrary substrates is important. Several methods were tried and a transfer process optimized for our purposes was established. To test and characterize the quality of our CVD graphene, we used optical and electron microscopy and Raman spectroscopy. Using our protocol, various devices to test the electrical properties of the transferred flakes have been fabricated. We measured the pH-sensitivity of a CVD graphene field effect transistor and it was found to be small, indicating a low defect density in the graphene [2].

As a next step, constrictions and small gaps in the graphene will be formed, using different approaches like state of the art lithography and direct patterning by a focused ion beam.

[1] X. Li et al., Science 324, 1312 (2009)

[2] W. Fu et al., Nano Lett. 11, 3597 (2011)

TUE 37

SiO₂/MgO – coated multiwall carbon nanotubes in polymer composites

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Because of their high aspect-ratio and strength MWCNTs are expected to be perfect

polymer reinforcement materials. Proper inorganic coverage on their surface might help to reduce the aggregation of CNTs and also to overcome consequent dispersability problem. Polymer filler materials – e.g. dolomite or talc – are often used in the industry to improve mechanical properties. In this work MWCNTs were coated with talc-like oxides to facilitate their incorporation into polyamide matrix. Silica-magnesia mixed oxides were synthesized from TEOS and magnesia salts ($\text{MgCl}_2 \times 6 \text{H}_2\text{O}$, $\text{Mg}(\text{NO}_3)_2 \times 6 \text{H}_2\text{O}$, $\text{MgSO}_4 \times 7 \text{H}_2\text{O}$) by the sol-gel method. As-prepared materials were characterized by TEM, SEM, Raman spectroscopy and XRD. Results showed that using $\text{Mg}(\text{NO}_3)_2$ mixed oxide coating formed on the surface of MWCNTs after annealing. In order to investigate the change of polymer's properties these samples were impregnated into polyamide matrix. Mechanical and thermal (melting and crystallization) properties of the composites were determined.

TUE 38

Preparation and photocatalytic properties of ZnO/MWNT nanocomposites

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Zinc oxide (ZnO) nanoparticles have been successfully deposited onto multiwalled carbon nanotubes (MWNT) templates for the preparation of new composite materials by a direct impregnation technique under different solvent conditions. Due to their high catalytic activity in the photodegradation of organic pollutants ZnO nanoparticles are of great interest. It is hoped that the new composite materials will have a synergic effect on both physical and chemical properties. The structure of ZnO nanoparticles can be controlled by changing the pH of the Zn precursor solution used in the preparation of the composites. ZnO-MWNT nanocomposites were characterized using TEM, SEM, RAMAN, XRD, TGA techniques. The photocatalytic activity of the as-prepared nanocomposite materials was also investigated in the gas-phase decomposition of EtOH. These experiments revealed that the nanocomposite has higher photocatalytic activity than the MWNT free ZnO nanoparticles.

TUE 39

Investigation of diameter selectivity of reductive hydrogenation on single-walled carbon nanotubes

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Reductive hydrogenation of different single-walled carbon nanotubes (HiPco, P2 and CoMoCat) were carried out. The samples were investigated by wide-range optical ($30\text{--}52000\text{ cm}^{-1}$), Raman and photoluminescence spectroscopy as well as by thermogravimetry-mass spectrometry.

On hydrogenation the reductive agent was melted potassium. Potassium dopes the nanotube bundles, the cations can enter the bundles and exfoliate them, making further doping easier. Since potassium is added in excess, the nanotubes are overdoped, all become metallic. These overdoped nanotubes are the starting material for hydrogenation (hydrogenating agent is methanol).

Normally, the higher the curvature of the nanotube, the higher the strain in its sp^2 -carbon framework, so the reactivity increases with the curvature. In our case, where doped nanotubes act as starting material of the reaction, the determining property in product distribution is not the curvature but the electronic structure of the doped nanotubes. This means that overdoping depends on the bandgap which becomes narrower with diameter. This causes a reverse reactivity which was confirmed by optical, Raman and photoluminescence spectroscopy.

TUE 40

Hopping transport in disordered fullerene films

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The charge-carrier mobility in organic semiconductors is the critical parameter that governs the performance of electronic devices. Low cost film fabrication techniques such as printing and solution processing generally result in disordered film structures, where charge carrier transport occurs by hopping between localized states. Therefore charge carrier mobility in these films is typically relatively low and strongly dependent on electric field, carrier concentration and temperature. Charge transport in disordered fullerene (C60) films in diode and field effect transistor geometry

is studied. Meyer-Neldel rule, typically observed in numerous temperature activated processes in nature, is observed in both types of devices. Both carrier concentration and electric field govern the activation energy for electron mobility in C60 films. Effective Medium Approach model is used to explain the experimental observations. It is shown that carrier concentration dependent mobility arises from fill-up of the low energy localized states within the DOS, while electric field dependence is a result of lowering the Coulomb barrier between neighbor hopping states by an external electric field.

TUE 41

Easy synthesis of Pd fullerene polymer structures from the molten state of tris(dibenzylideneacetone)dipalladium(0)

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Pd fullerene composites have been first synthesized and studied in the early 90's by for example Nagashima et al. In this study we present a novel solvent free approach. Even though utilizing initially toluene as solvent we can clearly show that the Pd fullerenes form during a heating step of the dry phase making it possible to apply direct coatings on substrates. We show that the Pd fullerene polymer phase forms at temperatures around the melting point of Pd_2dba_3 and that it proceeds upon further annealing which releases dba. We can thereby synthesize composites consisting of pure Pd fullerenes. The synthesis reactions were studied in TGA/DSC. TEM revealed that the material easily collapses under the electron beam into nanoparticles. Under very low doses almost no particles can be found. Raman confirmed the Pd fullerene polymer but showed a highly increased signal from pristine C_{60} when irradiated by high laser power. CVD experiments have been conducted on directly coated Si substrates showing similar results than earlier with Pd C_{60} catalysts giving further insight into the process. We believe that the approach is applicable for broad spectra of CVD experiments.

TUE 42

Iodine-doped Metallic Single-Wall Carbon Nanotubes

Elena D. Obraztsova¹, Alexander A. Tonkikh¹, Ekaterina A. Obraztsova¹, Ivan A. Nikitskiy¹, Igor V. Vorob'ev¹, Laurent Alvarez², Jean-Louis Bantignies², Jean-Louis Sauvajol²

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Separation of single-wall carbon nanotubes (SWNTs) onto semiconducting and metallic fractions is becoming more and more important. The semiconducting SWNTs

are needed for applications in transistors and non-linear optical elements, while the metallic ones are necessary for formation of transparent conductive electrodes instead of the most popular today ITO (indium tin oxide) ones. There are two approaches for separation of semiconducting and metallic nanotubes – to grow the necessary type [1] or to get it after a post-growth treatment of arbitrary nanotubes [2]. In this work we have formed the completely metallic fraction after doping of HiPCO SWNTs with iodine. The optical spectroscopy data (a suppression of E11 band in the UV-vis-NIR absorption spectrum and a broadening of the tangential mode in the Raman spectra) have confirmed the theoretical prediction about transformation of all nanotubes into metallic phase after doping. The transport measurements are in progress. The work was supported by RFBR 11-02-90731, and by the Russian President Grant for young scientists. 1. M. He et al., J. AM. CHEM. SOC. 132 (2010) 13994. 2. A. I. Chernov et al. Phys. Status Solidi B 246 (2009) 247

TUE 43

Dispersion, Assembly and Characterisation of Nitrogen-doped SWCNT devices

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¹School of Computer Science, The University of Manchester, UK

²Centre for Mesoscience and Nanotechnology, The University of Manchester, UK

³Department of Applied Physics and Center for New Materials, Aalto University, Espoo, Finland

In this poster, we describe the complete process including growth, dispersion, assembly and characterization of N-doped SWCNTs. N-doped single-walled carbon nanotubes (SWCNTs) were produced by floating catalyst CVD method with NH_3 as N-dopant source introduced into the gas-feed. Three different dopant levels were produced by varying the NH_3 concentration, at 0 ppm (undoped), 50 ppm and 100 ppm. The dry N-doped nanotube powder was then dispersed in NMP by multiple stages of ultrasonication, centrifugation and dilution. Ultimately, a stable dispersion was produced using identical processing for all three doping levels. Absorption spectroscopy was used to determine the concentration of these solutions. Subsequently, the N-doped nanotubes were deposited from solution on top pre-fabricated electrode arrays using dielectrophoresis (DEP). The DEP was optimised to yield individual N-doped nanotubes in each device for subsequent characterization. The N-doped SWCNT devices were characterised by Raman spectroscopy and electronic transport measurements to reveal the influence of doping on the electronic properties.

TUE 44**Perforated graphite: synthesis, structure and properties.**

Alexander V. Okotrub¹, Lyubov G Bulusheva¹, Vyacheslav Tur¹, Igor Asanov¹, Evdokiya Bushueva¹, Anton Gutakovskii², Andrey Chuvilin³

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³CIC nanoGUNE Consolider, San Sebastian

The controlled reduction of graphite oxide C₂O in a high-boiling inorganic or organic liquid at the temperature higher than 200°C proceeds with liberation of CO₂. As the result the initial graphite oxide transforms in a layered structure with high quantity of vacancy defects (holes) in the graphene sheets. The characteristic size of the holes is about 2 nm. The obtained perforated graphite materials were characterized by high-resolution transmission electron microscopy, scanning atomic-force microscopy, X-ray diffraction, Raman and optical absorption spectroscopy, and near-edge X-ray absorption fine structure. The materials have good electrical conductivity and porosity. The reactivity of the perforated graphite toward fluorination and oxidation was studied. The material possesses the high reversible electrochemical specific capacity at the lithium insertion and the high sensitivity to gases.

TUE 45**Spin-transport in carbon nanotubes: the role of dopants**

Andrea Pani¹, Niall McEvoy², Georg S. Duesberg², Nicole Grobert³, Vojislav Krsitić¹

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³Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK

Carbon nanotubes have been successfully employed as building blocks for spintronic devices [1]. Furthermore the possibility of doping carbon nanotubes gives them new properties, i.e. the presence of dopants can be exploited favourably to control the spin-transport mechanism. Studies on N-doped carbon nanotubes [2] have indicated an enhancement of the spin-orbit interactions, which is of key-relevance for the spin-control by externally applied electric fields (spin-field-effect-transistor).

The goal of this project is to provide a comparative study of doped and undoped multi-walled carbon nanotubes transport properties exploring the mK temperature region and in presence of strong magnetic fields (up to 12T).

Doped and undoped multi-walled carbon nanotubes have been dispersed onto a functionalized SiO₂ substrate and contacted with Ni electrodes by electron-beam lithography. These devices have been imaged with AFM and I-V characteristics at

room temperature have been acquired.

[1] L. Hueso et al., *Nature*, 445, 410 (2007)

[2] V. Krstić et al., *Europhys. Lett.*, 77, 37001 (2007)

TUE 46

TiO₂/WO₃/Au/CNT composite materials for photocatalytic hydrogen production

Zsolt Pap^{1,2,4}, Éva Karácsonyi³, Lucian Baia⁴, Lucian Pop^{2,4}, Virginia Danciu², Klára Hernádi⁵, Károly Mogyorósi³, András Dombi¹

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TiO₂/WO₃/Au/CNT composite materials were obtained using commercial TiO₂ (Anatase, Rutile and Aeroxide P25) and WO₃. The gold nanoparticles were deposited on the semiconductor oxides' surface by chemical reduction using sodium borohydride, and the CNT's were associated to the composite (in different concentrations 0.1-10 percent) by applying an ultrasonication method. The obtained nanocomposites were successfully characterized by several techniques including X-ray diffraction, transmission electron microscopy (TEM), etc. The aim of the present work was to find the best synthesis method and the optimal composition (i.e. carbon nanotube and gold content) of the composite for photocatalytic hydrogen production using oxalic acid as a sacrificial agent.

TUE 47

Plasma modified photoactive electrospun nanofiber materials

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²Institute of Physics of the ASCR, v.v.i., Prague, Czech Republic

Herein we present the study on effect of plasma treatment on photochemistry of electrospun polymeric nanofiber materials prepared from polystyrene (PS), polyurethane (PUR) and polyamide 6 (PA6) doped with 5,10,15,20-tetraphenylporphyrin (TPP) photosensitizer. Effect of plasma treatment on morphology and photochemistry was studied via microscopic methods, steady-state and time-resolved fluorescence, and absorption spectroscopy. Iodide method was used to measure the

quantum yields of photo-produced singlet oxygen. Photo-bactericidal activity of all nanofiber materials was evaluated against *E. coli*.

TUE 48

Influence of the molecular conjugation on the charge transport in anthracene derivatives

Mickael L. Perrin¹, Hennie Valkenier-Van Dijk², Jos S. Seldenthuis¹, Christian A. Martin¹, Jan M. van Ruitenbeek³, Jan C. Hummelen², Diana Dulić¹, Herre S. J. van der Zant¹

¹Kavli Institute of Nanoscience, Delft University of Technology, Delft

²Stratingh Institute for Chemistry and Zernike Institute for Advanced Materials, University of Groningen, Groningen

³Kamerlingh Onnes Laboratory, Leiden University, Leiden

Here, we present the electronic transport measurements through a series of single molecular wires. By using three different anthracene derivatives, we investigate the influence of the molecular conjugation on the charge transport. We compared current-voltage characteristics (IVs) of the linear conjugated anthracene wire to the cross-conjugated anthraquinone and the non-conjugated diHydro-anthracene wire using the mechanically controllable break junction technique in vacuum and at cryogenic temperatures. By fine-tuning the electrode spacing, we study the influence of the metal/organic interface on the molecular energy level alignment and the charge transport across the molecular junction. Depending on the junction configuration, we can access various transport regimes, which exhibit rich IV spectra. Using a tight-binding model approach, we can qualitatively understand some of the observed spectroscopic features.

TUE 49

Gap opening in graphene antidot lattices

E. C. Peters¹, A. J. M. Giesbers¹, M. Burghard¹, K. Kern^{1,2}

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The potential of graphene for future electronic applications and its fundamental physics has attracted extraordinary attention. However, the absence of a band gap in graphene has posed strong limitations on the development of technologically relevant graphene-based devices. One possibility to overcome this problem is the formation of graphene nanoribbons, either as isolated nanostructures or as an interconnected array within a graphene sheet, e.g. in the form of a twodimensional periodic array of nanoholes. While experimental studies have confirmed the opening of a band in gap in such graphene antidot lattices with neck widths of the order of 20

nm, a systematic understanding of the connection between their electron structure and the geometry of the holes has not yet been attained. Here, we explore in detail the gap opening behavior of graphene nano-meshes of different geometries under applied magnetic field. At low magnetic fields, the charge transport is governed by a soft Coulomb gap associated with Efros-Shklovskii variable range hopping, while at moderate fields there is a crossover to Mott VRH. At high B-fields a thermally activated gap emerges due to spin splitting effects.

TUE 50**Effect of Chemical Functionalization on the Thermoelectrical Properties of Single Walled Carbon Nanotube Networks**

Mingxing Piao¹, Urszula Dettlaff-Weglikowska¹, Siegmund Roth¹

¹School of Electrical Engineering, Korea University, Seoul

Carbon nanotube networks showing high electrical and low thermal conductivity are considered as a promising material for thermal energy conversion applications. However, the experimental thermoelectric figure of merit, ZT , of pristine carbon nanotubes indicating the possibility of a practical application is in the range of 10^{-3} - 10^{-2} instead of 2, typical for the standard thermoelectric materials like Bi_2Te_3 . In this work, we demonstrate the effect of the chemical treatment on the electrical conductivity and the Seebeck coefficient of the single walled carbon nanotube papers. Chemicals increasing the electrical conductivity due to the p-type doping show a decrease of the Seebeck coefficient. Whereas the neutrally, in terms of doping, acting polymers such as PVDF, PMMA, PVA, PS and PC, expected to reduce the thermal conductivity, slightly increase the Seebeck coefficient up to $94 \mu\text{V/K}$, the n-type dopants change the sign and the value of the Seebeck coefficient from $85 \mu\text{V/K}$ to $-74 \mu\text{V/K}$. A combination of these two type materials may open up the possibility of building flexible thermoelectric modules with a significantly improved thermoelectric performance.

TUE 51**Tip-enhanced Raman spectroscopy of multilayer graphene on gold substrate**

Emanuele Poliani¹, Janina Maultzsch¹

¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin

Localized surface plasmons (LSPs) can be used to achieve sub-wavelength spatial resolution in optical spectroscopy experiments such as Surface Enhanced Raman Spectroscopy (SERS) and Tip-Enhanced Raman Spectroscopy (TERS). In our TERS setup a tip-metal cavity is formed creating coupled modes of photons and plasmons, called gap modes. Gap modes are strongly localized inside the cavity with a consequent local enhancement of the electric field. In addition to the inelastic scattering of LSPs with the specimen inside the cavity, characteristic of its vibratio-

nal properties, a wide background is observed and interpreted as the emission of the resonant cavity [1]. The experimental system formed by an electrochemically etched Au tip and the Au substrate is studied in a TERS setup with side illumination. We investigate the interaction between multilayer graphene and the resonant cavity as well as localized emission of defects and inner unknown molecules. This preliminary study aims at understanding the interactions between gold and graphene, which is relevant e.g. in graphene electronic devices if gold is used as contact.

[1] B. Pettinger, K. F. Domke, Phys. Rev. B 76, 113409 (2007)

TUE 52

Thermal Expansion of Carbon Nanocoils

Zoran P. Popovic¹, Milan Damnjanovic¹, Ivanka Milosevic¹

¹Faculty of Physics, University of Belgrade, Serbia

Carbon nanotubes with helical geometries are experimentally observed by Zhang et al. in 1994. Their geometrical structure is described by four parameters: tubular diameter, pitch, inclination angle and diameter of a coil.

Experimentally investigations confirm that regularly coiled structure has periodic incorporations of pentagons and heptagons into their basic hexagonal carbon network. We consider a model of single wall nanotube pulled on a helix. Theoretically, problem of pentagons and heptagons distribution is solved with help of graph theory. Application of the line group symmetry enables efficient calculations of the relaxed configurations.

Coefficients of thermal expansion of carbon nanocoils are calculated by minimizing the Helmholtz free energy at finite temperature, and results are compared with those for straight carbon nanotubes. This study is based on molecular dynamic, using inter-atomic potential for carbon.

TUE 53

New insight on C–H–O ternary diagram for diamond growth by CVD linear antenna microwave plasma process

Štěpán Potocký¹, Oleg Babchenko¹, Tibor Ižák¹, Karel Hruška¹, Alaxander Kromka¹

¹Institute of Physics, Academy of Science of the Czech Republic, Prague

The process parametric window for diamond deposition using the CVD at low pressures is quite limited where addition of oxygen in the gas phase broadens this window. The lower boundary of the lens shaped domain in C–H–O ternary diagram concurs with the H₂–CO tie-line ($C/(C+O)=0.5$).

In this work we present the set of experiments where ratio of $C/(C+O)$ was kept constant at value 0.385. Effect of hydrogen concentration (ratio $O/(O+H)$ changed from 0.047 to 0.364) on plasma characteristics and deposited NCD films was investigated. Other process parameters in the linear antenna MW plasma CVD process

Tuesday, March 6th

Poster session

were kept constant, i.e. microwave power 1700 W, gas pressure 0.1 mbar, substrate temperature ≈ 540 °C. Raman spectroscopy confirmed the diamond character for all samples. Change of film morphology and grain sizes are assigned to the varied gas mixture (O/(O+H) resp. H/(H+C) ratios). Similarly, a transformation from film to diamond nanowire-like features is observed. The proposed growth model is correlated to optical emission spectroscopy measurements.



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FT-IR

- 08:30 – 09:30 **R. Schlögl, Berlin**
Functional groups on nanocarbons
- 09:30 – 10:00 **D. Guldi, Erlangen**
Tuning the electronic structure of low dimensional nanocarbons by means of charge transfer
- 10:00 – 10:30 **Coffee break**
- 10:30 – 11:00 **J. Englert, Fürth**
Reductive Exfoliation of Graphite and Covalent Functionalization of Graphene
- 11:00 – 11:30 **M. Strano, Cambridge**
Advances in understanding Chemistry of Graphene and Carbon Nanotubes: Fundamentals and Applications
- 11:30 – 12:00 **A. Turchanin, Bielefeld**
From organic monolayers to carbon nanomembranes and graphene with tunable structural, chemical and electrical properties
- 12:00 – 17:00 **Mini-Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **G. Güntherodt, Aachen**
Spin transport in graphene
- 19:00 – 19:30 **I. Grigorieva, Manchester**
Magnetism in graphene induced by point defects
- 19:30 – 20:00 **B. Feldman, Cambridge**
Unconventional Sequence of Fractional Quantum Hall States in Suspended Graphene
- 20:00 – 20:30 **R. Kawakami, Riverside**
Spin and Magnetism in Graphene

Wednesday, March 7th

Chemistry of CNT/graphene; magnetotransport

08:30**Functional groups on nanocarbons**Robert Schlögl¹¹Dept. Inorganic Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Nanostructured carbons, be they fullerenes, nanotubes/nanofibers or graphene all exhibit a large chemical anisotropy stemming from their structural anisotropy. All terminations exhibiting the basal plane orientation of graphite are only reactive to dispersive interactions with foreign species giving rise to adsorption or intercalation. Curved sp^2 -x surfaces exhibit the chemistry of localized double bonds favoring addition reactions. Prismatic terminations form with their dangling bonds covalent interactions leading to functional groups much alike those of substituted aromatic compounds. Local defects in any of these prototypical surface terminations enhance the variation in heteroatom terminations. This variety can lead to unexpected chemical properties that may be desired (catalysis, composite formation) or undesired (electronic properties, devices). The contribution discusses these qualitative differences, their consequences for chemical properties. It describes some of the spectroscopic and chemical characterization techniques. Despite many complementary techniques available the speciation of reactivity is still a complex challenge due to the manifold of functional groups.

09:30**Tuning the electronic structure of low dimensional nanocarbons by means of charge transfer**Dirk M Guldi¹¹University of Erlangen, Erlangen

I will discuss the implementation of a small molecule approach as well as an oligomer approach towards self-ordering / self-assembling semiconducting carbon nanotubes and / or graphene to realize functioning charge transfer materials that unify light harvesting, charge separation, and catalysis. In particular, our interlocking approaches involve design, materials, characterization, advanced measurements, and device fabrication. All of them are based on a broad range of spectroscopic and microscopic techniques and are meant to address the tuning of the electronic structure semiconducting carbon nanotubes and / or graphene by means of charge transfer / doping interactions. The composite nature of the resulting functional nanocarbons raises the exciting possibility of nanoscale charge transfer material having a tunable structure that can be tailored to a particular electronic functionality.

10:30**Reductive Exfoliation of Graphite and Covalent Functionalization of Graphene**

Jan M. Englert¹, S. Schmitt², K. C. Knirsch¹, P. Vecera¹, B. Butz³, S. Christiansen², E. Spiecker³, F. Hauke¹, A. Hirsch¹

¹Institute of Advanced Materials and Processes (ZMP), Friedrich-Alexander University Erlangen-Nuernberg, Dr.-Mackstr. 81, Fuerth

²Max-Planck Institute Erlangen, Günther Scharowsky-Str. 1, Erlangen

³Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander University Erlangen-Nuernberg, Cauerstr. 6, Erlangen

Functional graphene architectures are gathering increasing attention in the emerging field of covalent graphene chemistry. In order to preserve the option of reaching the stage of large scale processing of these materials we developed versatile reductive wet chemical bulk functionalization protocols.[1,2] In contrast to the oxidative exfoliation of graphite, the addition of excess electrons does not cause damage to the σ -scaffold of the graphene lattice. We repeatedly exfoliated single layer reduced graphene from different types of graphite with varying efficiency. In a second step we successfully used these activated graphene solutions[3] for covalent functionalization by electrophiles. Moreover, we developed statistical analytical tools for a detailed analysis of not only the functionalization products but also of the pristine graphene sheets produced after solvolysis. Herein, low levels of disorder in those graphenes on scales exceeding micrometers were found, outperforming typical values on oxidized materials.

[1] J. M. Englert et al., Nat.Chem. 2011, 3, 279

[2] J. M. Englert et al., Angew. Chem. 2011, 123, A17

[3] A. Catheline et al., Chem.Comm. 2011, 47, 5470

11:00**Advances in understanding Chemistry of Graphene and Carbon Nanotubes: Fundamentals and Applications**Michael S Strano¹¹Massachusetts Institute of Technology, Cambridge

Our lab at MIT has been interested in how the 1D and 2D electronic structure of carbon nanotubes and graphene respectively influences their chemistry. We demonstrate a solution-phase technique for the production of large-area, bilayer or trilayer graphene from graphite, with controlled stacking and characterize transistors generated from such materials. We also show a stark difference in the rate of electron transfer chemistry with aryl diazonium salts on monolayer graphene supported on a broad range of substrates. Reactions proceed rapidly when graphene is on SiO₂ and sapphire, but negligibly on alkyl-terminated and hexagonal boron nitride surfaces. Reactivity imprint lithography (RIL) is demonstrated as a technique for spatially patterning chemical groups on graphene by controlling the underlying substrate. We will also introduce several new concepts in sensor mechanisms utilizing carbon materials for the label free detection of protein-protein interactions, H₂O₂, NO and glucose, as well interfacing sensor arrays to live cells. Ion channels fabricated from the interior of a carbon nanotube have also been pioneered in our laboratory, as we have shown that single molecule, stochastic detection of individual ions is possible.

11:30**From organic monolayers to carbon nanomembranes and graphene with tunable structural, chemical and electrical properties**Andrey Turchanin¹¹Physics of supramolecular systems and surfaces, University of Bielefeld, Bielefeld

Two-dimensional (2D) carbon-based materials have been suggested for applications ranging from nanoelectronics to nanobiotechnology. Bottom-up approaches via molecular self-assembly have great potential to facilitate these applications. In this talk, I will report on the fabrication and characterization of carbon nanomembranes and graphene sheets made by electron-radiation induced cross-linking of organic self-assembled monolayers (SAMs) and their subsequent annealing. In this process, the SAM is converted into a homogenous nanocrystalline graphene sheet with well-defined thickness and arbitrary dimensions. Electric transport data demonstrate that this transformation is accompanied by an insulator to metal transition that can be utilized to control electrical properties such as conductivity, electron mobility and ambipolar electric field effect of the fabricated 2D carbon sheets. The suggested route opens broad prospects towards the engineering of advanced 2D carbon materials with novel physical and chemical properties on various solid substrates and on holey substrates as suspended nanomembranes.

18:30**Spin transport in graphene**Gernot Güntherodt¹¹Physics Institute (IIA), RWTH Aachen University, Aachen

Spintronics is shifting interest to carbon-based materials, such as graphene, because of high carrier mobilities, negligible spin-orbit coupling (SOC) and long spin relaxation lengths(1). Pure spin currents, holding the potential of low dissipation, are generated by separating the spin injection current-path from the E-field-free spin-potential detection path. For mechanically exfoliated bilayer graphene samples we found spin relaxation times at room temperature and low temperature of 2 ns (2), which are an order of magnitude longer than previously reported values (1). Similar values are reported in Ref. (3). However, these values are still way below the theoretically predicted ones ($\mu\text{s} - \text{ms}$) (4), because of, e.g., charged impurities introducing local SOC effects. Related random magnetic Rashba fields give rise to spin relaxation, which we identified as of the D'yakonov-Perel'-type. It implies longest spin relaxation times for the lowest mobilities, challenging spintronics devices.

- (1) N. Tombros et al., Nature (London) 448, 571 (2007). (2) T.- Y. Yang et al., Phys. Rev. Lett. 107, 047206 (2011). (3) W. Han and R. K. Kawakami, Phys. Rev. Lett. 107, 047207 (2011). (4) C. Ertler et al., Phys. Rev. B 80, 041405 (2009).

19:00**Magnetism in graphene induced by point defects**

Irina V. Grigorieva¹, R.R. Nair¹, M. Sepioni¹, I-Ling Tsai¹, O. Lehtinen², A. V. Krasheninnikov², J. Keinonen², A. K. Geim¹

¹School of Physics and Astronomy, University of Manchester, Manchester, UK

²Department of Physics, University of Helsinki, Finland

The possibility to induce magnetic response in graphene by introduction of defects has been generating much interest, as this would expand the already impressive list of its special properties. To date there have been many theoretical studies predicting that point defects in graphene should carry magnetic moments and these can in principle couple (anti)ferromagnetically. However, experimental evidence for such magnetism remains both scarce and controversial. In my talk I will review our recent experimental results where we show that point defects in graphene – (i) fluorine adatoms and (ii) irradiation defects (vacancies) – carry magnetic moments with spin $\frac{1}{2}$. Both types of defects lead to notable paramagnetism but no magnetic ordering could be detected down to liquid helium temperatures. The induced paramagnetism dominates graphene's low-temperature magnetic properties, despite the fact that maximum response we could achieve was limited to one moment per approximately 1000 carbon atoms. This limitation is explained by clustering of adatoms and, for the case of vacancies, by losing graphene's structural stability. Our work clarifies the controversial issue of graphene's magnetism.

19:30**Unconventional Sequence of Fractional Quantum Hall States in Suspended Graphene**Benjamin E. Feldman¹, Benjamin Krauss², Jurgen H. Smet², Amir Yacoby¹¹Department of Physics, Harvard University, Cambridge, MA 02138, USA²Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

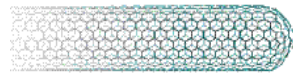
Graphene provides a platform to study unique many-body effects due to the relativistic nature of its charge carriers and the fourfold degeneracy that arises from their spin and valley degrees of freedom. We report local electronic compressibility measurements of a suspended graphene flake performed using a scanning single-electron transistor. Between filling factors $\nu = 0$ and 1, our measurements reveal incompressible fractional quantum Hall states that follow the standard composite fermion sequence $\nu = p/(2p \pm 1)$ for $p \leq 4$. In contrast, between $\nu = 1$ and 2, incompressible behavior occurs only at $\nu = 4/3, 8/5, 10/7$ and $14/9$. These fractions correspond to a subset of the composite fermion sequence involving only even numerators, suggesting a robust underlying symmetry. We also extract the energy gap of each fractional quantum Hall state as a function of magnetic field. The states at $\nu = 1/3, 2/3, 4/3$, and $8/5$ are strongest at low field, and persist below 1.5 T. The unusual sequence and relative strength of each fractional quantum Hall state provide insight into the interplay between electronic correlations and SU(4) symmetry in graphene.

20:00**Spin and Magnetism in Graphene**Roland K Kawakami¹¹Department of Physics and Astronomy, University of California, Riverside, Riverside, CA

Graphene is an attractive material for spintronics due to the low intrinsic spin-orbit coupling, low hyperfine coupling, and high electronic mobility. This introduces the possibility of a spin transport material with long spin lifetimes and long spin diffusion lengths. Experimentally, the gate-tunable spin transport at room temperature has been achieved with spin diffusion lengths of several microns, which makes it a unique and promising material for spin transport. I will report our latest results on spin transport such as efficient spin injection using smooth tunnel barriers, comparison of single-layer and bilayer graphene, and investigations of the origin of spin relaxation in graphene.

Graphene is also extremely interesting as a magnetic system where unusual properties of defect-induced magnetism, gate-tunable magnetism, and Kondo effect have been predicted. A controversial issue is whether defects such as hydrogen/fluorine adsorbates and lattice vacancies generate magnetic moments. I will present recent experiments that show a clear signature of magnetic moment formation through their spin-flip scattering (i.e. spin relaxation) of pure spin currents.

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Graphene transport; CNT/graphene applications

Thursday, March 8th

- 08:30 – 09:00 **R. Gorbachev, Manchester**
Graphene / Boron Nitride Heterostructures
- 09:00 – 09:30 **M. Calandra, Paris**
Phonon-mediated superconductivity in graphene by lithium deposition
- 09:30 – 10:00 **D. Elias, Manchester**
Electronic properties of free-standing graphene at low energies.
- 10:00 – 10:30 **Coffee break**
- 10:30 – 11:00 **C. Berger, Atlanta**
Epitaxial graphene nanoribbons
- 11:00 – 11:30 **M. Engel, Eggenstein-Leopoldshafen**
Light-matter interaction in a microcavity-controlled graphene transistor
- 11:30 – 12:00 **T. Weitz, Ludwigshafen**
Electronic properties of organic materials: small molecule field-effect transistors and graphene
- 12:00 – 17:00 **Mini-Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **M. Endo, Nagano**
Catalytically Grown Carbon Nanotubes
- 19:00 – 19:30 **A. Rinzler, Gainesville**
Single wall carbon nanotube based electronic junction control devices
- 19:30 – 20:00 **R. Martel, Montreal**
Probing Charge Transfer and Photothermoelectric Responses from SWNT Devices
- 20:00 **Poster III**

Thursday, March 8th

Graphene transport; CNT/graphene applications

08:30**Graphene / Boron Nitride Heterostructures**

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This presentation gives a brief overview of our previous studies, but is mainly focused on the fabrication and transport properties of multilayer boron nitride/graphene heterostructures. We study devices, where two independently contacted graphene sheets are separated by a layer of boron nitride. When brought close, two layers affect each other. For large carrier densities in one of them, the adjacent layer no longer exhibits a minimum metallic conductivity at the neutrality point, and its resistivity diverges at low temperatures. The observed localization is possible due to suppression of electron-hole puddles such that the carrier concentration can be low enough to satisfy $\lambda_F \sim l$. Close proximity also leads to frictional coupling between 2DEGs, giving rise to drag effect, which exhibits unusual behaviour beyond the scope of the previously studied ‘weakly interacting regime’. In addition, tunnelling between two graphene layers through a BN crystal was studied as a function of BN thickness and Fermi level position in both layers. The heterostructures can possibly be used as vertical field effect transistors.

09:00**Phonon-mediated superconductivity in graphene by lithium deposition**Francesco Mauri¹, Gianni Profeta², Matteo Calandra¹¹IMPMC, Université Pierre et Marie Curie - Paris 6, Paris²Università degli Studi di L'Aquila, Italy

Graphene is the physical realization of many fundamental concepts and phenomena in solid-state physics. However, in the list of graphene's many remarkable properties, superconductivity is notably absent. If it were possible to find a way to induce superconductivity, it could improve the performance and enable more efficient integration of a variety of promising device concepts. To this end, we explore, by first-principles DFT calculations, the possibility of inducing superconductivity in a graphene sheet by doping its surface with alkaline metal adatoms [1], in a manner analogous to which superconductivity is induced in graphite intercalated compounds (GICs). As for GICs, we find that the electrical characteristics of graphene are sensitive to the species of adatom used. However, unlike GICs, we find that lithium atoms should induce superconductivity in graphene at a higher temperature than calcium.

[1] G. Profeta, M. Calandra, F. Mauri, arXiv:1105.3736, to be published in Nature Physics.

09:30**Electronic properties of free-standing graphene at low energies.**Daniel Elias¹¹The School of Physics and Astronomy, The University of Manchester, Manchester

Graphene samples inhomogeneities and broadening of the energy levels due to finite lifetime of the charge carriers prohibited the direct access to the most interesting regime of zero electron and hole concentrations. A significant improvement of the quality of graphene samples has been achieved by removing the underlying substrate. After annealing, such free-standing graphene devices can present mobilities of the order $10^6 \text{cm}^2/\text{Vs}$ and charge inhomogeneities less than 10^9cm^{-2} . This allowed us to study the electronic spectrum of graphene at very low energies, close to the Dirac point. Therefore, we have performed transport and magnetotransport measurements in free-standing graphene devices, and have experimentally observed a reconstruction of the energy spectrum of monolayer graphene, driven by the renormalizations of the Fermi velocity due to electron-electron interactions. In the bilayer samples, we have also found the low energy parabolic dispersion to be replaced by multiple electron and hole pockets with linear dispersion. This spectrum is strongly modified in magnetic field, which is an evidence of an interaction driven phase transition.

10:30**Epitaxial graphene nanoribbons**

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To develop graphene transistors, graphene functionalization or confinement in narrow ribbons is used to create a gap in otherwise gapless graphene. But patterning techniques severely degrade graphene, and measured transport gaps have been associated with Coulomb blockade and localization effects. We have developed a technique [1, 2] to directly grow graphene ribbons on silicon carbide substrate step edges at high temperature. These nanoribbons, down to 10 nm width, do not require post-growth damaging lithographic processing. Contrary to lithographically patterned ribbons, there is no evidence for a gap. Transport data indicate reduced edge scattering and ballistic transport. This opens the way to epitaxial graphene device architectures beyond diffusive electronics.

[1] M. Sprinkle, et al., Nature Nanotechnology 5, 727, (2010).

[2] W. A. de Heer et al. PNAS 108(41), 16900 (2011).

11:00**Light-matter interaction in a microcavity-controlled graphene transistor**Michael Engel¹¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe

Here we report the monolithic integration of a graphene transistor with a planar optical microcavity. We find that both photocurrent generation as well as electrically excited, thermal light emission of graphene can be controlled by the spectral properties of the microcavity. The device constitutes a first implementation of a cavity-enhanced graphene light detector, as well as a demonstration of a fully integrated, narrow-band thermal light source. Most importantly, the optical confinement of graphene by the microcavity profoundly modifies the electrical transport characteristics of the integrated graphene transistor. The modifications of the electrical transport can be related to the microcavity-induced enhancement or inhibition of spontaneous emission of thermal photons. The concept of optical confinement of graphene enables a new class of functional devices as, for example, spectrally selective and highly directional light emitters, detectors, and modulators. Moreover, it opens up the opportunity for investigating fundamental, cavity-induced modifications of light-matter interactions in graphene.

Thursday, March 8th

Graphene transport; CNT/graphene applications

11:30

Electronic properties of organic materials: small molecule field-effect transistors and graphene

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The electronic properties of organic materials depend strongly on the interplay of various factors: the characteristics of the individual molecules, their processing conditions and the interface to other materials used in the same system (e.g. in a field-effect transistor). We will give an overview from applied topics such as the structure-property relationship of polycrystalline small-molecule films for use in field-effect transistors all the way to details on symmetry-broken states of bilayer graphene.

18:30**Catalytically Grown Carbon Nanotubes**Morinobu Endo¹¹Shinshu University, Nagano

Carbon nanotubes have attracted lots of attention from various fields of scientists because of their extraordinary physical and chemical properties and their nano-sized one-dimensional nature. The dominant way of synthesizing carbon nanotubes is a catalytic chemical vapour deposition (CCVD) method using iron particle. Noticeably, highly crystalline and pure carbon nanotubes are industrially produced through the right combination of the CCVD and the subsequent high-temperature thermal treatment. In addition, a CCVD method using iron nanoparticles enabled us to produce single-, double- and multi-walled carbon nanotubes. Herein, the controlled growth of high-purity carbon nanotubes based on the CCVD method is described, and then their current usages in the range from multifunctional filler in various matrices as well as in electrochemical systems such as lithium ion battery will be discussed with a detailed study of the effect of nanotubes texture and morphology. Finally, the biocompatibility study on carbon nanotubes will be described, because the evaluation of toxicity and the risk control are essential issues for successful business of carbon nanotubes. I envisage that carbon nanotube will contribute enormously to the environmental and energy era of the 21st century.

19:00**Single wall carbon nanotube based electronic junction control devices**Andrew G. Rinzler¹¹University of Florida, Gainesville, FL, USA

The low density of electronic states of the SWNTs implies large shifts of their chemical potential, and thus their work function, depending upon their charge state. Since the work function line-up across the interface between two materials dictates the junction transport properties, the ability to tune the SWNT work function provides a new degree of freedom for tuning electronic transport. We initially considered chemical charge transfer doping as one means to achieve such junction engineering but soon became intrigued by the idea of using field gating for an electronically tunable control over the trans-junction transport. That led to a radical redesign of the organic thin film transistor to a vertical architecture that exploits SWNTs as a field gated source electrode. The architecture readily lent itself to making a vertical *light emitting transistor* which defines a new state of the art in such devices. In another direction we also realized junction control in a SWNT/n-Si Schottky junction solar cell, enhancing performance by 30%. These developments and latest progress will be discussed.

19:30**Probing Charge Transfer and Photothermoelectric Responses from SWNT Devices**Richard Martel¹¹RQMP and département de chimie, Université de Montreal, Montreal, Canada

Charge transfer doping by molecules such as atmospheric gases are ubiquitous phenomena influencing the properties of carbon-based devices. By using single-walled carbon nanotube (SWNT) layers and graphene sheets as testbeds, we investigated the impact of different gases on the field-effect switching of both nanoscale and thin-film devices. The talk will present results highlighting the important role of redox active species such as the water/oxygen couple. Unintentional p-doping of graphene layers as well as a drastic suppression of n-type conduction in SWNTs are good examples illustrating the impact of air exposure. In other sets of experiments, we explored covalent functionalization onto the NT sidewall in order to build new interfaces between molecules and nanotubes. The covalent bonding was used to gain selective optical and electrical probing of NTs and to derive novel electronic and optical functions. Finally, we will describe the photovoltage (PV) properties of SWNT layers when exposed to local illumination. Dominated by photothermoelectric effects, the PV response can be used to extract the doping profiles and local Seebeck coefficients of SWNT layers.

THU 1**Impurities in Graphenes and Carbon Nanotubes**Martin Pumera¹¹Chemistry and Biological Chemistry, Nanyang Technological University, Singapore

CNTs contain a large amount of residual metal-catalyst impurities which are practically impossible to remove even after treatment with strong acid at elevated temperatures. It was also shown that such impurities can completely dominate many properties that were originally attributed to CNTs.

These impurities can alter electrochemical properties, influence redox properties of biomarkers, have effects on adsorption properties and can also cause adverse toxicological effects.

Here we discuss this and we also show that metallic impurities in graphenes prepared from graphite can dramatically influence their properties

THU 2**A local optical probe for measuring motion and stress in a nanoelectromechanical system**Antoine Reserbat-Plantey¹, Laëtitia Marty¹, Olivier Arcizet¹, Nedjma Bendiab¹, Vincent Bouchiat¹¹Institut Néel, CNRS et Université Joseph Fourier, BP 166, F-38042 Grenoble Cedex 9, France

Nanoelectromechanical systems can be operated as ultrasensitive mass sensors and ultrahigh frequency resonators and can also be used to explore fundamental physical phenomena such as nonlinear damping and quantum effects in macroscopic objects. Various dissipation mechanisms are known to limit the mechanical quality factors of nanoelectromechanical systems and to induce aging due to material degradation, so there is a need for methods that can probe the motion of these systems, and the stresses within them, at the nanoscale. Here, we report a non-invasive local optical probe for the quantitative measurement of motion and stress within a nanoelectromechanical system based on Fizeau interferometry and Raman spectroscopy. The system consists of a multilayer graphene resonator that is clamped to a gold film on an oxidized silicon surface. The resonator and the surface both act as mirrors and therefore define an optical cavity. Fizeau interferometry provides a calibrated measurement of the motion of the resonator, while Raman spectroscopy can probe the strain within the system and allows a purely spectral detection of mechanical resonance at the nanoscale. ARP et al Nat. Nano. accepted

THU 3**AC TEM of graphene defects and their evolution under electron beam irradiation**

Alex W. Robertson¹, Christopher S. Allen¹, Yimin A. Wu¹, Jamie H. Warner¹

¹Materials Department, University of Oxford, Oxford, United Kingdom

The atomic structure of defect configurations in graphene are of interest due to their inevitable effect on the local band structure. High resolution aberration corrected transmission electron microscopy (AC TEM) images of defects in chemical vapour deposition (CVD) grown single layer graphene are used to help determine the atomic configuration and stability of various defects. The fine image resolution allows for the atomic structure of the defects to be readily distinguished. Multislice TEM image simulations are used to corroborate the determined defect structures. The evolution of the defects under electron beam irradiation was used to evaluate their relative stabilities.

THU 4**Photoluminescence evolution of filled semiconducting nanotubes**

Philip Rohringer¹, Xianjie Liu¹, Marianna V. Kharlamova¹, Paola Ayala¹, Thomas Pichler¹, Takeshi Saito²

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²AIST, Tsukuba, Japan

Here we present studies on the evolution of the optical properties from single-walled carbon nanotubes (SWNTs) due to filling of the host material, using photoluminescence (PL), optical absorption and Raman spectroscopy. For biomedical applications, SWNTs have to be in a biocompatible solution, however, such a procedure normally quenches the luminescence signal because of charge transfer from the surfactant molecules to the nanotube. This effect can again be compensated by filling the hollow core of the nanotube with various materials. In this study, we used DIPS SWNTs with a broad diameter distribution and filled them with metallocenes. A strong enhancement of the PL signal can be seen for nanotubes with optimal diameters for the as mentioned charge transfer compensation. Later on, these tubes were transformed to double walled nanotubes (DWNTs). Only few DWNT show a PL response for the inner tubes, with an overall decrease of the signal. This is attributed due to an interaction and/or charge transfer to the outer tubes. Funding by the FWF is greatly acknowledged.

THU 5**Width-dependent effects in edge-functionalized armchair graphene nanoribbons**

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Edge passivation has been shown to strongly influence the fundamental properties of graphene nanoribbons (GNRs). We present ab initio calculations of hydroxy functionalized armchair GNRs (AGNRs) of different widths and find the band-gap to be greatly reduced in N -AGNRs with $N = 3p + 1$ and increased in all other ones [1]. This behavior is driven by two independent effects. On the one hand, hydroxy passivation imposes axial strain on the ribbon structure which in turn modifies the band-gap depending on which family the given N -AGNR belongs to. Moreover, the addition of hydroxy groups to the ribbon edges results in a weakened quantum confinement of the electronic wave function in all AGNRs. We furthermore study the functionalization-induced shift of characteristic phonons, i.e. the LO and TO modes and the breathing-like mode in AGNRs of different widths. Especially the large downshift of the TO in principle allows for an experimental determination of the degree of functionalization.

[1] N. Rosenkranz *et al.*, PRB 84, 195438 (2011)

THU 6

A high energy spectroscopic study on the absorption of NO₂ on metallicity separated single walled carbon nanotubes

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Single walled carbon nanotubes (SWCNTs) are promising components of gas sensors considering that the adsorption of gases on their walls can modify their electronic transport properties. Although, SWCNT-based systems are nowadays set as high sensitive sensors in presence to several chemical species, the interaction of toxic molecules associated to their intrinsic metallic character is still elusive. In this work, we report a study on the photoemission and x-ray absorption response of purely metallic and semiconducting SWCNTs film and buckypaper as a function of increasing NO₂ dosage up to several 100 Langmuir. Both film and buckypaper samples were found to bind NO₂ via physisorption and weak chemisorption. The adsorption is strongly temperature dependent. We also observed that other species such as -NO and NO₃- were produced by light induced chemical interaction during synchrotron experiments. The saturation dose for the metallic tubes is about twice as much gas as compared to the semiconducting ones. This highlights that conduction electrons play also an important role in the sensitivity to adsorbed gases.

Work supported by FWF and EU Proposal N° 20105285 for ELETTRA.

THU 7**Enhancement of optical properties of CVD graphene by integration with photonic crystal**

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A considerable potential of graphene is contemplated for photonic and optoelectronic applications, where the combination of its unique optical and electronic properties can be fully exploited: a linear dispersion of Dirac electrons in graphene is a distinctive feature which makes this material ideal for a wide spectral range and ultrafast saturable light absorption. In this contribution we propose to combine graphene layers with Photonic Crystal (PC) Si membrane slabs, in order to enhance optical absorption of the former, thus opening the way to new types of ultra-fast saturable absorber photonic devices, operating at low incident optical energy flux. We have described a CVD method developed for graphene synthesis. Graphene samples with a controlled amount of layers have been prepared and transferred onto different substrates. The optical characterization of devices has been based on the measurements of the reflectivity spectra of the devices, which reveals the temporal confinement characteristics of the PC structures and directly indicates the amount of absorption enhancement of the graphene layers, induced by the PC Si membrane layer.

Work supported by RFBR 10-02-00792-a

THU 8**Analytical expression for valence band structure of iodine spirals inside carbon nanotubes**

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Various experimental investigations show that carbon nanotubes can act as “nanocontainers” which form unique one-dimensional structures inside. Iodine can be crystallized inside a carbon nanotube in form of spirals with the geometry depending on the tube diameter [1,2]. In the present work the electronic band structure of such one-dimensional spirals was calculated within a tight-binding approach. The screw symmetry was applied to derive an analytical expression for the valence bands corresponding to a range of realistic structure geometries. The interaction parameters were fitted to reproduce the DFT results for a linear iodine chain. The obtained expression can be used to determine the dependence of the electronic structure on

the spiral geometry and to estimate the Fermi energy shift of a structure composed from an iodine spiral and a carbon nanotube.

The work was supported by RFBR and RAS research projects.

1. Fan, X.; Dickey, E. C.; Eklund, P. C.; Williams, K. A.; Grigorian, L.; Buczko, R.; Pantelides, S. T.; Pennycook, S. J. *Phys. Rev. Lett.* 2000, 84, 4621.
2. Lunhui Guan, Kazu Suenaga, Zujin Shi, Zhennan Gu, and Sumio Iijima *Nano Lett.* 2007, 7, 1532.

THU 9

A Resonance photoemission study of the electronic structure of metallicity sorted ferrocene filled SWCNT

Markus Sauer¹, Hidetsugu Shiozawa¹, Paola Ayala¹, Georgina Ruiz Soria¹, Xianjie Liu¹, Alexander Chernov¹, Hiromichi Kataura², Katsuhiro Yanagi², Stefan Krause³, Thomas Pichler¹

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Single-walled carbon nanotubes (SWCNT) filled with metallocenes have proven to be an interesting topic especially because the tunability of nanotube properties could prove useful in future electronic applications. We studied SWCNT films as well as bucky paper filled with ferrocene where mixed and for the first time metallicity sorted tubes were used as basic material. By heating the samples to temperatures of up to 900°C the ferrocene filled SWCNT are converted into Fe-filled double-walled carbon nanotubes (DWCNT). X-ray absorption spectroscopy reveals this transition by showing the change in the Fe 2p absorption. Furthermore we show a resonant photoemission study on the Fe 2p edge where we compare the ferrocene features with previous studies on pure Fe and thereby analyse the charge transfer from the ferrocene to the nanotubes and its change upon conversion into DWCNT. Additionally the hybridization effects are studied in detail. Finally transport measurements directly show the change in charge transfer upon heating by monitoring the difference in conductivity.

Funding by the FWF and the European Community's Seventh Framework Programme is greatly acknowledged.

THU 10

Resonant Raman scattering of single- and bilayer molybdenum disulfide

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Atomically thin layers of molybdenum disulfide (MoS_2) can be produced by mechanical exfoliation from the bulk material, comparable to graphene. Due to their band gap of approximately 1.9 eV, the lack of dangling bonds and strongly enhanced photoluminescence compared to the bulk, thin layers of MoS_2 appear ideal for novel electronic and optoelectronic devices. For this purpose it is a key requirement to understand their electronic and vibrational properties. We present Raman resonance profiles of the first-order Raman modes in the energy range of the first optical transition. We show that in resonance the A_{1g} mode in bilayer MoS_2 has a more than five times higher Raman intensity than for monolayer MoS_2 . This result is important with respect to the determination of the layer number using Raman spectroscopy, since a linear behavior between the layer number (up to 4 layers) and the Raman intensity is generally assumed. Furthermore we present $\hat{A}\mu$ -photoluminescence of MoS_2 samples covering a wide range of layer numbers.

THU 11

Grafting carbon nanotubes on carbon fibers: Influence of the growth parameters on the mechanical properties

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Carbon nanotubes (CNTs) have attracted particular interest as nano-additives in carbon fiber-reinforced polymer composites. Most potential of CNTs is seen in improving the damage resistance of these materials. An interesting way of CNTs integration is growing CNTs directly on the surface of carbon fibers, to obtain so-called CNT-grafted carbon fibers. However, the main drawback of this approach is the degradation of the tensile strength of carbon fibers, which originates from the high growth temperatures used during the catalytic Chemical Vapor Deposition (CVD) process as well as from the damage caused by the catalyst/carbon fiber interaction. In the present work, we studied systematically the growth of CNTs on PAN-based carbon fibers by means of catalytic CVD technique. By varying the growth conditions, the effect of various parameters has been investigated in detail. Particular attention is paid to the equimolar $\text{C}_2\text{H}_2\text{-CO}_2$ reaction, which allows CNT growth at much lower temperatures. The effect of the grafting process on the mechanical properties of the carbon fibers is investigated by single-fiber tests before and after catalyst deposition, and after the CNTs growth.

THU 12**Controlled aggregation-deaggregation dynamics of single walled carbon nanotubes through photo-switchable dendritic surfactants**

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Here we will present our results on the use of a new class of smart surfactants made out of a conformational molecular switch able to tailor and affect the properties of carbon nanotubes just by light exposure. Our results on the reversible light-triggered deaggregation-reaggregation dynamics of single-walled carbon nanotubes will be shown and attention will be devoted to the achievement of the light-driven control of the state of the SWNT suspension. The surfactant contains an azobenzene core connected to an alkyl chain, for an improved debundling ability, and a glycerol dendron, for ensuring solubility in water. This ensures compatibility for bio-oriented applications; the light-induced deaggregation mechanism could lead to a controlled transport and local targeted release of molecules of biological interest, which could open the way to a new use of carbon nanotubes as drug carrier.

THU 13**A resonance Raman study of C-chain@DWCNTs**

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Here we present a resonance Raman study of linear carbon chains inside double-walled carbon nanotubes (C-chain@DWCNTs) prepared by high-temperature annealing of DWCNTs with thin inner tube. The characteristic resonance Raman response of linear carbon chains is observed at around 1850cm⁻¹ and exhibits a maximum for yellow/green laser excitations. Compared with the Raman spectra of other C-chain@CNTs, we find that these carbon chains inside CNTs, whether the carbon chains are long or short, inside SWCNTs, DWCNTs or MWCNTs, with hydrogen atom dangling bonds or not, show a very similar resonance Raman characteristics. These characteristics can be used as a fingerprint for linear carbon chains and confirm the structure of C-chain@CNTs complementary to a direct observation by HRTEM. This also allows us to monitor the evolution of the modified response of metal/molecular-chain@CNTs. Funding by the CSC and FWF is greatly acknowledged.

THU 14**Influence of the surfactants on the performance of SWCNT thin film transistors**

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Semiconductor enriched single wall carbon nanotubes (s-SWCNTs) have a great potential for the channel material of thin film transistors (TFTs). However, actual device performance is depending on the deposition procedure of thin film. For example, some kinds of surfactants have been used for preparation of aqueous solution of s-SWCNT, but it is still not clear how the surfactant affects the thin film formation and namely the transport properties. To clarify this issue, we focused on the sort of surfactant to be the best for thin film formation. In this work, we tried 4 kinds of surfactants, sodium dodecyl sulfate (SDS), sodium cholate (SC), sodium deoxycholate (DOC), and sodium dodecylbenzene sulfonate (SDBS). Thin films were prepared with common dip, dry and washing procedure and then morphology was characterized using atomic force microscopy. Thick bundles were frequently observed in the films prepared by SDS and SDBS, while very thin bundles are dominant in the case of SC and DOC. It was found that these topological differences give great influence on the transport properties of the TFTs. High on/off and high mobility were easily obtained in cases of SC and DOC.

THU 15**Spontaneous formation of symmetric carbon nanostructures in a confined environment**

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Self-organisation of matter is essential for natural pattern formation and chemical synthesis. Modern material science seeks further developments on the production of quality new materials with advanced functionalities based on nanostructures. Our research focuses on understanding and control of nanoscale self-organisation via studies of novel processes to the production of carbon nanostructures. Self-pressured synthesis, in particular, uses a pure organometallic gas to produce novel symmetric nanostructures[1]. The process performed within a sealed vessel at elevated temperatures allows high-pressure molecules to react with each other in a free-standing manner, allowing novel symmetric carbon nanostructures to emerge spontaneously. The growth symmetry is determined at a given temperature and pressure, allowing the phase diagram for a precursor to be produced. In particular, at pressures that exceed 5 MPa mirrored nano-spirals are produced. A mathematical approach based

on continuum equations taking into account mass conservation and chemical composition quantitatively explains the shape evolution. [1] H. Shiozawa, et al. Nano Lett. 11,160–163 (2011).

THU 16

NMR spectroscopy, the Tomonaga-Luttinger liquid state, and the magnitude of the hyperfine coupling in SWCNTs

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We report ¹³C NMR measurements on ¹³C-enriched SWCNTs. The temperature dependence of the nuclear spin-lattice relaxation rate (SLRR) exhibits a power law variation, as expected for a Tomonaga-Luttinger liquid (TLL) [1]. We develop the theory of the SLRR for a TLL and show that it is orders of magnitude enhanced when compared to a Fermi-liquid with the same density of states. Analysis of the SLRR data confirms the usual small, $\leq 1 \mu\text{eV}$ value of the hyperfine coupling constant in SWCNTs [2]. This is in clear contradiction to the transport data on SWCNT quantum dots [3], where a huge, orders of magnitude larger than usual, hyperfine coupling constant was reported.

[1] Y. Ihara, P. Wzietek, H. Alloul, M. H. Ruemmeli, T. Pichler, and F. Simon, EPL 90, 17004 (2010).

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[3] H. O. H. Churchill, A. J. Bestwick, J.W. Harlow, F. Kuemmeth, D. Marcos, C. H. Stwertka, S. K. Watson, and C. M. Marcus, Nat. Phys. 5, 321 (2009).

THU 17

Periodically grown Sexithiophene/Para-hexaphenyl nano-fibres

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It has been demonstrated that organic-organic heteroepitaxy of sexithiophene(6T)

on top of highly parallel oriented para-hexaphenyl (p-6P) nano-fibers can be successfully implemented. By the chosen approach 6T is forced to align parallel to the p-6P template molecules, which yields highly polarized emission of both species. It has been shown that the fabricated structures provide two different 6T emissions which originate from interfacial and crystalline 6T molecules. Within this contribution we report about the epitaxial growth of periodic p-6P/6T multi-layer hetero-structures on top of p-6P nano-fibers. By a periodical deposition of 6T monolayers and p-6P spacers it is demonstrated that the strongly polarized spectral contribution of interfacial 6T can be precisely controlled and amplified whereas crystallization of red emitting 6T phase is successfully suppressed. Moreover, it is demonstrated by morphological investigations provided by atomic force microscopy (AFM) and fluorescence microscopy that periodical deposition of 6T leads to a significant improvement concerning emission and morphological nano-fiber homogeneity.

THU 18**Mesoscopic Conductance Fluctuations in graphene**

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We studied Mesoscopic Conductance Fluctuations (MCFs) in suspended as well as on substrate placed graphene crystals of mesoscopic size, which are visible in transport characteristics up to relatively high temperature (70 K). Under perpendicular magnetic (B) and electric (VG) fields, randomly distributed quantum dots form along the sample due to inhomogeneity of charge carrier density. In transport measurements, the localized states in quantum dots cause MCFs, reflecting particle interactions with surprising sensitivity. A map of these MCFs in the plane B vs VG exhibits exotic states with fractional filling factors. The temperature dependence of MCF-amplitude decay also indicates that the origin of the MCF is related to localized states within quantum dots. However, rather unusual exponential decay is often observed, when the MCF features overlap.

THU 19**Bottom-up fabrication and electronic properties of graphene nanoribbons**

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Its remarkable properties make graphene attractive for use in nanoscale devices. However, graphene is semimetallic and thus not directly suitable for most electro-

nic or optoelectronic devices, which require a semiconductor with a specific, finite bandgap. This can be overcome by structuring graphene on the nanometer scale, which opens a bandgap suitable for room-temperature applications. A fundamental structure is the graphene nanoribbons (GNR), a narrow strip of graphene, whose electronic and optical properties vary as a function of size and shape. Experimentally, nanostructured graphene and graphene-related materials are accessible via lithographic techniques or chemical treatment, but both methods are limited with respect to their ultimate resolution and precision. We will show how these limitations can be overcome by using a bottom-up strategy, allowing the atomically precise fabrication of GNRs. Furthermore, we will present recent results on the electronic properties of sub-nanometer GNRs.

THU 20**Growth of Individual Carbon Nanotubes with Precise location**

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Electronic devices or sensors based on individual single walled carbon nanotube (SWNT) remain at the prototype level. This is the consequence of the limited reliability of the Chemical Vapour Deposition (CVD) processes (low yield and impurities) and the absence of control of the electrical properties of the SWNT obtained. The lack of specificity of the SWNT positioning is also a major limitation. To improve the location and narrow the electronic property distribution of the SWNTs, best strategy relies on the precise deposition of one single catalyst particle with controlled size. We have developed a method based on e-beam lithography. A negative tone resist is doped with Co. After patterning resist dots, the metal is segregated at 800°C and the amorphous carbon generated by the decomposition of the resist is etched. At the end of the process, individual particles with a diameter of $1.2 \pm 0.2 \text{ nm}$ are localized within an area of 80 nm^2 , corresponding to the surface of the lithographed dot. High-quality SWCNTs are grown with a diameter of $1.2 \pm 0.25 \text{ nm}$ by CVD from ethanol. The parametric study performed to optimize the catalyst deposition and SWNT growth process will be presented.

THU 21**Excitonic resonances in WS_2 nanotubes**

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As the first member of the family of inorganic nanotubes (INT), WS₂ NTs were synthesized in 1992. Owing to their triple layered structure there is considerably more strain involved in the bending of the layers than in CNTs and the diameters of INTs are hence much larger. Like in bulk WS₂, the first direct optical transitions are governed by excitons. Raman spectra of WS₂ NTs exhibit additional features as compared to the bulk spectra, most prominent among them a (LA+TA) mode. Here we present Resonance Raman profiles of single WS₂ nanotubes in the exciton energy region. In addition, Raman spectra of WS₂ NTs under hydrostatic pressure are analyzed.

The derived optical transition energies for the INTs lie below the value found for the bulk sample with an increasing redshift in exciton energy with decreasing diameter. Slightly different resonance conditions of the (LA+TA) and the A_{1g} Raman modes of WS₂ result in a non monotonic change of the (LA+TA)/A_{1g} ratio with excitation energy. This change can also be followed in Raman spectra of WS₂ NTs under hydrostatic pressure and can be explained in terms of a pressure induced gradual bandgap opening.

THU 22

Alkali-doped MoSI nanowires: charge transport in single bundles

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Mo₆S_{9-x}I_x (MoSI) family of molecular nanowires exhibits unique molecular scale functionality in terms of flexibility and connectivity to gold and peptide groups due to sulfur atoms bridging molybdenum octahedra and terminating the nanowires. This favours use of MoSI in molecular electronics as covalent molecular interconnects. However, being intrinsically semiconductive, their application is currently hindered by their relatively low conductivity.

By exposing Mo₆S₃I₆ to Na or K vapour we manage to introduce free carriers into nanowires, which show no morphological changes under SEM. Their magnetic susceptibility resembles Pauli paramagnetism, however with a very low saturation field. Their conductivity increases by many orders of magnitude, up to 10⁵ S m⁻¹. Temperature dependence of DC conductivity of single nanowire bundles in different circuits reveals several transport mechanisms ranging from Luttinger liquid to Coulomb blockade or ohmic conductance with negligible temperature dependence in the range from room temperature to 70 K. When exposed to air the dopant ions which seem to be weakly bound begin to form oxides on a timescale of several minutes.

THU 23**Investigation of carbon nanotubes and silica mesopores filled by NaNO_2 ferroelectric**Elena Stukova¹, Aleksandr S. Fedorov², Dmitry A. Fedorov²¹Amur State University, Blagoveschensk²L.V. Kirensky Institute of Physics of RAS, Krasnoyarsk

Filling of carbon nanotubes (CNT) and silica mesopores by NaNO_2 order-disorder ferroelectric is investigated both theoretically and experimentally. In experiments it is shown that the filling leads to permittivity increase by 1-2 orders of magnitude compared with the bulk ferroelectric and can reach 10^5 value at frequency of 1 MHz. By DFT-GGA calculations using VASP package it is shown that narrow semiconductor CNT filling by the NaNO_2 also leads to essential permittivity increase at different frequencies and to high Born effective charges. Calculations of potential barriers for NaNO_2 elementary dipoles flip inside CNT show that they are lower and the ferroelectric switch is quicker than in the case of bulk ferroelectric. In general we can say that CNT and silica mesopores filled by the NaNO_2 ferroelectric can be perspective as high permittivity materials or as switching elements in future electronic devices.

THU 24**Core level binding energies of defected and functionalized graphene**Toma Susi¹, Markus Kaukonen¹, Mathias Ljungberg², Paola Ayala³, Esko I. Kauppinen¹¹NanoMaterials Group, Department of Applied Physics, Aalto University School of Science, Finland²Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, E-08193 Bellaterra, Spain³Faculty of Physics, University of Vienna, Austria

X-ray photoelectron spectroscopy (XPS) is a widely used tool for probing carbon-based nanomaterials. To interpret the binding energies measured by XPS, references to which such energies can be compared are needed. We employed core-hole calculations using a Delta Kohn-Sham total energy differences method recently implemented [1] in the real-space grid-based projector-augmented wave (GPAW) DFT code to calculate reference core level energies for defected and functionalized graphene. We calculated the C1s and O1s core energies for simple oxygen and hydrogen functionalities such as the hydroxide, epoxide and carboxylic groups. In addition, we considered the elementary atomic defects: single and double vacancies, and the Stone-Thrower-Wales defect. Finally, modifications of the reactive single vacancy with O and H containing groups were considered. The calculated C1s and formation energies were compared to data in the literature, and Bader analysis employed to elucidate the effect of charge transfer to the observed shifts.

[1] M.P. Ljungberg, J.J. Mortensen, and L.G.M. Pettersson, J. Electron Spectros. Related Phenom. 184 (2011) 427

THU 25

Charge stabilization by reaction center protein immobilized to carbon nanotubes functionalized by amine groups and poly(3-thiophene acetic acid) conductive polymer

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A growing number of studies are giving clear indications that photosynthetic reaction center proteins (RC) bind successfully to nanostructures while retaining their functional activity. The main goal of current research activities is to find best systems and conditions for the photoelectric energy conversion as well as for the stability of these bio-nanocomposites. In our studies, RC proteins were immobilized through specific chemical bonding to amine functional groups and through conductive polymer (poly(3-thiophene acetic acid, PTAA)) attached to the multi walled carbon nanotubes (MWNT). Both structural (FTIR spectroscopy, TEM, AFM) and functional (absorption change and conductivity) measurements confirm the effective RCs binding to the functionalized MWNT. The kinetics of the light induced absorption change indicates that RCs remain active in the composite and interactions between the protein cofactors and the CNTs exist. The light generated photocurrent is also measured electrochemically in a modified cell design with transparent MWNT electrode.

THU 26

Electron spin resonance in superconducting boron doped diamond

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We study boron doped diamond (BDD) powders using electron spin resonance (ESR) spectroscopy. The samples are produced with microwave plasma assisted chemical vapour deposition (CVD) method and are characterized by resistivity, microwave conductivity, and Raman spectroscopy measurements. We identify three paramagnetic centers and, in addition, the ESR spectra in the 75 K to 300 K temperature range indicates the presence of a fourth ESR signal, which we tentatively assign to conduction electron spin resonance signal of BDD. The density of states (DOS) corresponding to itinerant electrons is determined from the calibrated ESR signal intensity. The experimental DOS agrees with the DOS values based on photoemission spectroscopy measurements. The validity of the Elliott-Yafet relaxation mechanism for BDD is discussed.

THU 27

Coronene and other PAHs for synthesis of graphene nanoribbons encapsulated in SWNTs

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Coronene can be considered as small piece of hydrogen terminated graphene, recently called as “nanographene”. Reaction of coronene polymerization was recently shown to be a road to synthesis of nanographenes with progressively large size [1]. Dimeric form of coronene (dicoronylene) can easily be synthesized by annealing above 800K while higher temperatures favor oligomerization into larger molecules. Confined polymerization and fusion of Polycyclic Aromatic Hydrocarbons (PAHs), coronene and perylene, in inner space of SWNTs allows to obtain novel material: graphene nanoribbons encapsulated in single-walled carbon nanotubes (GNR@SWNT) [2]. One-dimensional space inside nanotubes helps to align coronene or perylene molecules edge to edge to achieve dimerization and oligomerization of the molecules into long nanoribbons. The PAH fusion reaction provides a very simple and easily scalable method to synthesize GNR@SWNT in macroscopic amounts. 1. A. V. Talyzin, et al, J. Phys. Chem. C, 115, 13207, (2011) 2. A.V. Talyzin et al, Nano Lett., 11, 4352, (2011)

THU 28**Low-cost separation of metallic and semiconducting single-wall carbon nanotubes for mass production**Takeshi Tanaka^{1,2}, Satoshi Asano², Hiromichi Kataura^{1,2}¹Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Japan²Technology Research Association for Single Wall Carbon Nanotubes (TASC), Japan

For the electrical application of single-wall carbon nanotubes (SWCNTs), separation between metallic (M) and semiconducting (S) SWCNTs is required. We have developed various separation methods of M- and S-SWCNTs using agarose gel [1,2]. In these methods, column separation is superior in terms of simplicity, rapidity, scalability, automation, etc [2]. For the industrial mass-production of M- and S-SWCNTs, however, it is required to lower the cost of the separation further. Here we report the improvement of the M/S separation to obtain the separated SWCNTs at a low cost. Among the chemicals used in the column separation, the cost of the gel (Sephacrose, GE healthcare) and surfactants occupies the greater part of the total cost. We searched alternative gel and newly found an agarose-based gel which cost only about one-fiftieth of Sepharose gel. For the elution of the bound SWCNTs, sodium dodecyl sulfate with NaCl solution can also be used instead of sodium deoxycholate solution. These new separation condition enables us to save the separation cost drastically.

[1] Tanaka et al., Phys. Status Solidi RRL 2011, 5, 301

[2] Tanaka et al., Appl. Phys. Express 2009, 2, 125002

THU 29**Spatially resolved electronic structure of individual graphene grain boundaries**Levente Tapaszto¹, Peter Nemes-Incze¹, Gergely Dobrik¹, Kwon Jae Yoo², Peter Vancso¹, Geza I Mark¹, Chanyong Hwang², Laszlo P Biró¹¹ Institute for Technical Physics and Materials Science, Centre for Natural Sciences, Budapest, Hungary²Center for Advanced Instrumentation, Korea Research Institute of Standards and Science, Daejeon, Republic of Korea

Grain boundaries are ubiquitous in large-area CVD-grown graphene samples. These one-dimensional topological defects are expected to substantially alter the electronic properties of the ideal graphene lattice. In order to understand their behavior, experimental studies are required to clarify the mechanisms through which these structural defects affect the charge carrier propagation. Here, we investigate the electronic properties of individual graphene grain boundaries by scanning tunneling microscopy and spatially resolved tunneling spectroscopy measurements. Our

findings revealed that the conductivity inside the boundaries is significantly suppressed for both electrons and holes. Furthermore, graphene grain boundaries can give rise to n-type inversion channels within the overall p-doped graphene sheets, providing p-n junctions with sharp interfaces on the nanometer scale. These properties were found to be robust against structural disorder and to persist for grain boundaries of various atomic configurations. We compare these findings to the results of wave packet dynamical simulations on the charge carrier propagation and scattering across graphene grain boundaries.

THU 30

Reducing the diameter of vertically aligned single walled carbon nanotubes by Nitrogen doping: Synthesis and Spectroscopy study

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Chirality control is one of the major challenging goals to achieve unique properties of SWNTs. This can be indirectly sorted out through controlling the tube diameter to minimize number of chiralities. However, it requires the use of supporting materials which needs post-treatment to purify, and can also damage SWNTs. The growth on flat substrate is also required for some applications. The mean diameter of SWNTs synthesized on flat substrate is reduced significantly from 2.1 nm to 0.7 nm by using acetonitrile-mixed ethanol without changing the vertical alignment. Upon adding marginal amount of acetonitrile (1%), the 1 at.% incorporated substitutional graphitic sp² N content is detected and found to correlate with catalyst morphology independent diameter reduction and more likely for small-diameter SWNTs [1]. The absorption, Raman spectra and TEM clearly portrays the vast differences in the tube diameter.

[1] T. Thurakitseree et al. Carbon, submitted

THU 31

Wide range optical study on double-walled carbon nanotubes prepared from separated outer tubes

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Carbon nanotube chemistry continues to present intriguing possibilities in the nanoscience field. One of these is the encapsulation of small molecules or another nanotube in single-walled carbon nanotubes, another is the application of tubes

separated by electronic type (metallic and semiconducting). The same interest in the application of double-walled nanotubes – due to their diverse beneficial properties given by the characteristics of the outer tubes – can be observed. Combining these areas, we will report wide range optical studies on fullerene-filled separated carbon nanotube thin films, and we are also investigating how the electronic type of the outer nanotube affects the type of the created inner tube, when double-walled nanotubes are formed.

THU 32

Orientation selective tailoring of graphene edges using e-beam lithography and carbothermal etching

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The transport properties of graphene nanoribbons strongly depends on the quality and orientation of their edges. The reduction of edge roughness not only enhances the ribbon conductance, but such exotic transport features like the half-metallic behaviour of zigzag oriented nanoribbons are also expected to take place. In this work we investigate the combination of e-beam lithography (EBL) and the so-called carbothermal etching (CTE). During CTE [1] (a high-temperature annealing of patterned graphene on silicon-dioxide in a neutral atmosphere), the irregular edges of the graphene sheet are slowly etched away, forming edges parallel with the zigzag direction of the lattice. We have successfully created hexagonal holes in graphene using the aforementioned anisotropic etching method (CTE) from an antidot-lattice made by EBL and subsequent plasma etching. We also report on the low-temperature transport characterization of these samples. Our results show that CTE could serve as a fabrication step to improve the edge roughness of structures predefined by EBL and standard plasma etching.

[1] Nemes-Incze et al., Nano Research (2010) 3: 110–116, DOI 10.1007/s12274-010-1015-3

THU 33

Towards the control of the diameter of individualized SWCNTs in CVD process at low temperature

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It is well established that the diameters of SWCNT depend strongly of that of catalyst particles. The growth of SWCNTs with narrow size distribution is a real challenge because it needs to use perfectly calibrated catalyst particles with size close to 1 nm. In the current work we show that in fact it is possible to favour the selective growth of SWCNTs with a narrow diameter distribution on supported catalyst particles with a broad size distribution as ranged between 0.5 and 10.0 nm. The structure of carbon deposit has been controlled by managing the carbon feedstock, and by adjusting the rate of carbon formation on the surface of catalyst particle. At temperature lower than 600°C, only SWCNTs or carbon nanofibers were obtained, related to the synthesis parameters. Comparative analyses of SEM and TEM observations and Raman spectroscopy of isolated individual SWCNTs grown on silicon substrates allowed to show why the growth of MWCNTs with parallel walls seems to be difficult, and that it is possible to tailor the growth of SWCNTs with a narrow diameter distribution (0.5 to 1.5 nm) by limiting the catalytic activity of the largest catalyst particles.

THU 34

Nanomanipulation of Graphene using E-beam and Block Copolymers

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Generation of a customised electron bandgap in combination with a high carrier mobility is a key issue for electronic applications of graphene. One pathway studied recently for opening a bandgap is that of dense antidot lattices. While conventional top-down approaches are inadequate in terms of reaching the dimensions predicted to result in bandgaps of a useful size, self-assembled structures such as block copolymers can be used to deliver the ultrahigh density needed. Another application is programming of thermoelectric properties through manipulation of the electron and phonon transport lengths.

In the present work, several options for tuning the properties of graphene through nanopatterning are considered; direct structuring of graphene, and indirect modulation through nanopatterned surfaces. Apart from the direct influence of the periodic, alternating contact with polymer/substrate and air for partially suspended graphene, which can itself open a bandgap, it has been predicted that graphene may conform mechanically to a nanostructured surface, which should contribute to the electronic bandgap as well. Electrical and morphological measurements will be presented.

THU 35**Calculated Production Yields in Metallofullerene Series**Filip Uhlik¹, Zdenek Slanina², Shigeru Nagase²¹Charles University in Prague, Prague, Czech Republic²Institute for Molecular Science, Okazaki, Japan

Endohedral fullerenes are fascinating compounds where an atom or a small molecule is trapped inside the fullerene cage. They have several interesting applications, e.g., $\text{Gd@C}_{82}(\text{OH})_n$ can be used as a MRI contrast agent, $^{140}\text{La@C}_{82}$ can be used as a radiotracer, N@C_{60} can be used as a q -bit in quantum computers, etc. There are several ways how to prepare them, but for metallofullerenes the most important one is by the classical arc technique. The production yields, however, show a very complicated pattern, some compounds can be easily prepared, for others only spectra could be recorded, some were never observed. In this contribution we show how these observations can be rationalized on the basis of *ab initio* calculations and statistical thermodynamics and the relative production yields in homologous series can be successfully predicted.

THU 36**NANOCOMPOSITE MATERIALS: GROWTH OF CVD DIAMOND FILM ON BUCKY-PAPER SUBSTRATE**Marian Varga^{1,3}, Mario Kotlar^{1,2}, Viliam Vretenar², Tibor Ižák^{1,3}, Martin Ledinsky³, Alexander Kromka³, Marian Vesely¹¹Institute of Electronics and Photonics, FEI STU, Ilkovičova 3, SK-812 19 Bratislava²Danubia NanoTech, s.r.o., Ilkovičova 3, 841 04 Bratislava, Slovak Republic³Institute of Physics of the ASCR, v.v.i., Cukrovarnicka 10, Praha 6, 16253, Czech Republic

In this article we investigate the nanocomposite material formation, particularly the deposition of nanocrystalline diamond film on buckypaper substrate. The buckypapers were prepared from single-wall carbon nanotubes mixture produced by laser ablation method. A part of the buckypaper substrate was nucleated by ultrasonic treatment in nanodiamond suspension. The diamond deposition was carried out in hot filament chemical vapor deposition system. Scanning Electron Microscopy and Raman spectroscopy were used for the surface morphology analysis and characterization of carbon phases, respectively. After the deposition we observed the change of surface morphology from nanocrystalline diamond to carbon nanowalls character. Part of buckypaper substrate masked during deposition remained unchanged, while only the nucleated part exhibited the same morphology changes, which is discussed more detailed in the article.

THU 37**Reductive Functionalization of Graphene Using Modified Birch Conditions**Philipp Vecera¹, Jan M. Englert¹, Frank Hauke¹, Andreas Hirsch¹¹University of Erlangen-Nuernberg, Institute of Advanced Materials and Processes, Dr. Mack Strasse 81, Fuerth, Germany

The fabrication of graphene remains a highly challenging task particularly in large quantities. Since 2004, several production techniques were investigated coarsely divided into the top down and bottom up approach. Covalent bulk functionalization of graphene exhibits many hurdles for a wet chemical approach. Moreover, the outstanding properties of graphene can only be utilized if the sp^2 lattice retained mostly intact by converting basal carbon atoms from sp^2 to sp^3 hybridization during the functionalization sequences. Beyond that the introduction of functional groups, especially $-COOH$, may be used for the subsequent coupling of a broad variety of chemical entities. On the foundation of well-established SWCNT functionalization procedures, several different types of pristine graphites available from various vendors were investigated. A general reaction scheme based on modified Birch conditions in tetrahydrofuran is presented. By subsequent addition of various functional chemical groups, versatile functionalized graphene materials are obtained. Statistical Scanning Raman Microscope techniques reveal homogeneity and degree of functionalization of the materials.

THU 38**Suspensions of single-wall carbon nanotubes in binary polar solvents for optical power limiting**Anastasia Venediktova¹, Andrey Vlasov¹, Elena D. Obraztsova², Dmitry Videnichev³¹Dept. Chem., Saint Petersburg State University, Saint Petersburg²A.M. Prokhorov Institute of General Physics, Russian Academy of Sciences, 38, Vavilov Str., Moscow, 119991, Russia³S.I.Vavilov State Optical Institute, 12, Birzhevaya line, St. Petersburg, 199034, Russia

We report a study of fluid carbon nano-composites. The aim was getting a set of physical properties relevant for using the materials as the optical-power limiters. The type of the systems was: a suspension of single-wall carbon nanotubes (SWNT) stabilized with an amphiphile (sodium dodecylbenzenesulfonate, pluronic F-127 or ionic liquid dodecylmethylimidazolium chloride) in a binary polar medium (water solutions of glycerol, triethylene glycol, polyethylene glycol 400 or acetone). Employing binary solvents provided a broad temperature interval (down to $-50\text{ }^{\circ}\text{C}$) of the system stable fluidity, duration being over a year. All the systems have shown a good optical power limiting even in a pulse-repetition mode of applying to them laser radiation (532 nm): limiting factor ca 40. Noteworthy is their

promising bleaching resistance. We track an impact of the solvent viscosity, surface tension and dielectric constant as well as the dielectric optical function of the amphiphile micro-environment of SWNTs upon the non-linear optical properties of the composite. The work was supported by Russian Foundation for Basic Research (grants # 11-03-01106-a and #10-02-00792)

THU 39

Layering-controlled exfoliation of graphene and bottom-up integration into electronic devices

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Here, I present two approaches which yield high-quality, large sized flakes of pristine graphene in solution. In the first approach, HOPG is treated with H₂SO₄ and HNO₃, then rinsed with DI water and expanded by annealing. An intermediate graphite bisulfate is formed which decomposes readily in the presence of water to return the graphene to its pristine condition. This method yields high purity flakes of monolayer and multilayer graphene in solution.

While monolayer graphene has attracted the most attention, bilayers and trilayer graphene have very unique and exciting properties as well; however, large-scale controlled production of bilayers and trilayer graphene is lacking. I will present a novel solution-phase approach, whereby stage-controlled intercalation of graphene with inter-halogen compounds followed by expansion and dissolution can give solutions of mostly bilayers or trilayer flakes.

Once graphene flakes are in solution, bottom-up integration into pre-determined locations in an electronic circuit is a scalable and CMOS compatible way to produce graphene based electronics.

THU 40

Electrical conductivity of single-wall carbon nanotubes under high pressure

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According to recent experimental data, single wall carbon nanotubes (SWCNT) exhibit a sequence of phase transitions and demonstrate a high structural stability up to 35 GPa of non-hydrostatic pressure beyond which an irreversible transformation occurs. Here we report on the study of electrical properties of SWCNTs at pressures up to 40 GPa in the temperature range of 300 - 400K. High pressure was generated in diamond anvil cell. The anvils are made of electrically conduc-

ting "carbonadotype synthetic diamond. In the pressure range 10-25 GPa the CNT electrical resistance decreases considerably, whereas above 25 GPa it remains essentially unchanged. Such behavior of the resistance can be connected to a structural modification of the SWCNTs or/and change of the conductivity character at high pressure. Raman spectra of the samples recovered after 30 GPa exhibit a large increase of D/G band intensity ratio. Pressure dependences of resistance, activation energy for conductivity and charge carriers mobility were determined and analyzed.

THU 41

Nonlinear Optical Response of Two-Dimensional Silver Nanoparticles

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Two-dimensional Ag nanoparticles, e.g. triangular silver nanoplates (TSNP) [1], are known to have increased Surface Plasmon resonance which leads to strong nonlinear optical properties. Nonlinear saturable absorption is necessary for materials used as mode lockers in lasers to obtain light pulses with very short duration, in the order of femtoseconds. The lowest achievable absorption wavelength of TSNP is 511 nm having an edge length of 12 nm [1]. By increasing the size of the nanoplates a red shift of the absorption peak is achieved. Nonlinear optical properties are commonly studied by using the z-scan technique. Here, a thin sample is moved through the focus of a laser beam to vary the light intensity on the sample. This results in a change of the light absorption of the sample in case of an open aperture z-scan, or the refractive index when using the closed aperture setup.

In this study the nonlinear optical properties of Ag nanoplates in aqueous solutions were investigated using the z-scan method. Nanoparticles with different sizes and resulting absorption wavelengths were analyzed using a laser at constant excitation energy.

[1] D. Charles et al. Plasmonics 6 (2011) 351-362

THU 42

Momentum dependent electron energy loss in single- and multi- layer graphene

Philipp Wachsmuth¹, Michael K. Kinyanjui¹, Ralf Hambach¹, Jens Leschner², Gerd Benner², Ute Kaiser¹

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Our interest in collective electronic excitations (plasmons) in graphene is motivated by the need to understand its electronic structure, collective behavior and

potential applications in nano-plasmonics. We have applied angle-resolved electron energy-loss spectroscopy in a transmission electron microscope (TEM) to measure the momentum-dependent loss function of free-standing single- and multi-layer graphene. We have focused on energy-loss up to 40eV covering a momentum transfer range of $0 \leq q \leq 1.45 \text{ \AA}^{-1}$ along the $\Gamma - M$ and $\Gamma - K$ directions. In this energy range, the response of graphene to fast electrons is dominated by two high-energy plasmons, known as π - and $\pi - \sigma$ - plasmon respectively [1]. We will show the energy-momentum dependence (dispersion) of the π -plasmon peak as a function of the number of graphene layers. The dispersion of this π -plasmon changes from a linear behavior, in mono-layer graphene, to a parabolic, graphite-like behavior in 5-6 layers of graphene. These results are further discussed and compared to density functional theory calculations.

[1] T. Eberlein et al., Physical Review B, vol. 77, no. 23, Jun. 2008

THU 43

Piezoresistance of semimetallic carbon nanotubes

Christian Wagner¹, Jörg Schuster², Thomas Gessner^{1,2}

¹Center for Microtechnologies, Chemnitz University of Technology, Chemnitz

²Fraunhofer Institute for Electronic Nano Systems ENAS

We investigate the piezoresistive effect of carbon nanotubes (CNTs) within density functional theory (DFT) aiming at realistic semi-metallic CNTs. They are excellent candidates for the application in nano-electromechanical sensors (NEMS) due to their small bandgap at zero strain leading to a finite resistance at room temperature. The application of strain induces a bandgap-opening leading to a tremendous change in the resistivity.

DFT with the LDA- or GGA-approximation yields reasonable results for pure carbon systems like CNTs [1] and will be applied to calculate the electronic structure of experimentally relevant CNTs. Combined with the non-equilibrium Green's function theory (NEGF) DFT is used for transport calculations at finite bias voltage to obtain the conductivity of CNTs. We compare our DFT results for the resistivity of strained CNTs to results of analytic Tight-Binding models [2]. Future studies aim to the piezoresistive behavior of doped CNTs within the same framework.

[1] Tournus, F. & Charlier, J.-C., Phys. Rev. B, 2005, 71, 165421

[2] Kleiner, A. & Eggert, S., Phys. Rev. B, 2001, 63, 073408, Yang, L. & Han, J., Phys. Rev. Lett., 2000, 85, 154

THU 44

Self Assembling and Covalent Attachment of Oligo-Viologens on CNTs

Lorenz Walder¹, Shamaila Sadaf¹, Veronica-Alina Constantin¹, Liangcheng Cao¹

¹Institute of Chemistry, University of Osnabrück, Osnabrück

Semiconducting CNTs decorated with monomeric viologens (4,4'-bipyridinium salts)

have been reported to exhibit ambiently stable n-doping. We present here the modification of CNTs with new oligo- and polymeric viologens. The modifier compounds can be classified as follows: a) Triple-branched viologen stars consisting of up to 12 alternating di-benzyl- and di-phenyl-viologens,[1] b) di-phenyl-viologen rods with extended pi-conjugation over up to 6 nm, and c) on CNTs polymerized N-phenyl-N'-alkyl viologens. Clear evidence for the viologen wrapped CNTs is based on STM, electrochemistry and spectroscopy. Beside single CNT modification, the cross-coupling of CNTs by large viologen oligomers or polymers thereof is described. [1] V. A. Constantin et al., Eur. J. Org. Chem., 2012, 913-917

THU 45**Doped nanocrystalline carbon electrodes for graphene and CNT transistors**

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¹Nanoelectronics Materials Laboratory, Namlab, Dresden, Germany

²Technische Universität Dresden, Institute for Nanoelectronic Materials, Dresden, Germany

³Technische Universität München, Institute for Technical Electronics, Munich, Germany

⁴IFW, Leibniz Institute for Solid State and Materials Research, Dresden, Germany

The use of doped ohmic contacts for graphene nanoribbon (GNR) and carbon nanotube (CNT) transistors is projected to boost the on-currents and enhance performance for both digital and high frequency applications compared to the use of Schottky contacts [1]. In this work we study nanocrystalline doped carbon for use as source and drain electrodes for CNTs and graphene. Metallic carbon layers are deposited in a CMOS compatible chemical vapor deposition process as described in [2]. XRD and Micro-Raman revealed the composition of Sp² carbon flakes of typical sizes of 1.7 nm interlinked within an amorphous C matrix. In order to tune the work function, the carbon layers have been doped by two methods: a) post deposition anneal at 900°C in NH₃ and b) post treatment at 400°C with N radicals from a remote plasma source. In both cases photoelectron spectroscopy revealed a clear incorporation of nitrogen and the formation of C-N bonds. The impact of different work functions on the performance of CNT FETs will be discussed in detail.

[1] Youngki Yoon, Jing Guo et al. IEEE Transact Elec. Dev. 55, p. 2314 (2008)

[2] A. Graham et al. Journal of Appl.Phys. 107,114316(2010)

THU 46**In-situ TEM electrical and heat measurements exemplified on graphene membranes**

Benedikt Westenfelder¹, Tony Amende¹, Johannes Biskupek², Simon Kurasch², Ferdinand Scholz¹, Ute Kaiser²

¹Institute of Optoelectronics, Ulm University, Ulm

²Central Facility of Electron Microscopy, Ulm University, Ulm

An approach has been realized in order to study electronic properties of free-standing graphene at temperatures up to 1000 K in a transmission electron microscope (TEM). For this purpose a commercial Gatan TEM specimen holder (Model 628) has been modified such that 4 contacts are practically available for electrical measurements whereas 4 other contacts remain for heating and temperature sensing at one and the same small specimen volume (3 mm in diameter). With this extension electrical measurements and well-controlled specimen heating can be performed at the same time. The magnetic field of the microscope's objective lens was determined to be 1.2 T at 80 kV applying a custom-made Hall probe as TEM specimen. This one-time-only calibration procedure allows us to carry out Hall measurements at different temperatures. In first experiments graphene membranes have been suspended freely between four electrodes deposited on proper specimens. Simple characteristics on bi-layer graphene were measured inside the TEM for temperatures up to 500 K. This happened with and without simultaneous imaging in order to separate the effect of electron irradiation on adsorbed impurities.

THU 47

Production of Three-Dimensional Graphene Structures via Transfer Printing

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¹Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin

²School of Chemistry, Trinity College Dublin

Graphene has attracted much research interest due to its exceptional mechanical and electronic properties. The flexibility, high mobility, and transparency of the material make it very promising for future electronic applications. One of the major hurdles for this material is that single layer graphene possesses a zero-bandgap. A number of methods to open a band gap in graphene have been proposed; one of them is to use bilayer graphene. Measurements of handcrafted double layer graphene indeed show bandgap opening. However, a clear route to create bilayer graphene intentionally is yet to be developed.

We have developed a novel method to produce layered graphene structures using patterned elastomeric stamps. The structures have been characterised using techniques such as scanning probe microscopy and Raman spectroscopy. These structures can be applied to a range of substrates via transfer printing and have a wide variety of applications, including electrochemical cells and gas sensors.

THU 48**Investigation of Carbon-Silicon Schottky Barrier diode**

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¹School of Chemistry, Trinity College Dublin, Dublin

²Center for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin

The fabrication of high performing Schottky barrier diodes between silicon and two different types of conductive carbon films is reported. The diodes are fabricated by a simply spin coating and annealing of photoresist films (PPF) or by the chemical vapour deposition of pyrolytic carbon (PyC) onto n-type silicon wafers. After patterning and etching with a metal hardmask the current-voltage characteristics of Schottky barrier diodes were recorded. Using an extended thermionic emission theory taking account of series resistance of the substrate and the Norde function, the ideality factor (n), the barrier height and the series resistance were extracted. The ideality factors were $n=1.28$ for the PPF/n-Si diode and $n=1.44$ for the PyC/n-Si diode which are not far away from those of commercial products. Thus these highly durable and easily fabricated diodes may prove to be contenders for commercial products. Moreover, the diode characteristics can be used to evaluate the electrical properties of thin carbon films.

THU 49**Solvation of graphite oxide in different polar solvents**

Shujie You¹, Serhiy M. Luzan¹, Junchun Yu¹, Bertil Sundqvist¹, Alexandr V. Talyzin¹

¹Department of Physics, Umeå University, Umeå

Graphite oxide (GO) has attracted recently a lot of attention as a precursor for preparation of various graphene-related materials. One of the most interesting properties of GO is possibility to disperse it in solution on separate sheets and structural breathing connected to various degrees of hydration. However, so far most of GO structural studies were related to interaction of GO with water while almost any polar solvent is easily absorbed between GO sheets as well. Here we present results of synchrotron radiation XRD study of GO solvation with several polar solvents: methanol, ethanol, acetone and dimethylformamide (DMF). Structural properties of GO produced by Brodie method and immersed in excess amounts of these solvents were studied in a broad temperature interval using XRD and DSC. Solvation and desolvation of GO structure is found to be strongly affected by variations of temperature. The results obtained are of interest for solution related chemistry of GO and for reduction of GO into graphene which is often performed in various solvents.

THU 50**High Density Carbon Nanotube Growth using Plasma Pretreatments**C Zhang¹, R Xie¹, G Zhong¹, B Chen¹, J Robertson¹¹University of Cambridge, Cambridge

Carbon Nanotubes (CNTs) have some very promising uses such as interconnects and thermal interfaces which require high density CNTs. However, the CNT density achieved so far by chemical vapour deposition (CVD) is still limited by the catalyst particle density, because the catalyst is prone to agglomerate at typical CVD temperatures (500–700°C). A recent study showed that Co nanoparticles can be immobilized by a thin carbon layer before CNT growth in pulsed plasma CVD [1]. Here, we develop this process further. We employ 15s dc-plasma (1 W/cm², 3.5 mbar, 15–30% C₂H₂, 200–400°C) to deposit a carbon layer on top of a Al(10 nm)/Fe(1.5 nm) surface, prior to CNT growth in 4–8% C₂H₂ at 650°C without plasma. We find that the CNT mass density increases from 30 to ~110 mg/cm³, indicating higher area densities. This density is ~3 times larger than for forest grown with standard conditions. Further optimisation is under way. These results will have significant impact on CNT applications.

1.Y. Yamazaki et.al App. Phys. Exp. 3 (2010) 055002

THU 51**Atomic Scale Studies of Single-Walled Carbon Nanotube-Interactions with Transition Metal Clusters**Thilo Zoberbier¹, Johannes Biskupek¹, Ute Kaiser¹, Thomas Chamberlain², Elena Bichoutskaia², Navaratnarajah Kuganathan², Andrei Khlobystov²¹ZE Mat.Wiss. Elektronenmikroskopie, Universität Ulm, 89081 Ulm²School of Chemistry, University of Nottingham, University Park, Nottingham NG7 2RD, United Kingdom

Single-walled carbon nanotubes (SWNTs) have proven to be ideal containers for atomically resolved imaging of sub-nanometer molecule interaction dynamics. At a borderland between chemistry and physics they do not only feature a mandatory confinement of the reactants but also provide a unique environment for carbon-interaction and catalysis. In this work we study catalytically active metal-nanoclusters enclosed by SWNTs by means of aberration-corrected high-resolution transmission electron microscopy (AC-HRTEM) operated at an acceleration voltage below the knock-on damage threshold of the carbon structure. Under the effect of the electron beam and in dependence of its energy (20 keV to 80 keV) we observe diverse interactions of Os, Re and W nanoclusters with the nanotubes' inner sidewall which range from adhering to and moving along the sidewalls up to constricting and cutting the tubes by the clusters. Atomically resolved in-situ observations of these interactions finally give rise to a detailed description of the underlying processes using an physicochemical approach. This way the interaction mechanisms as well

as the dependence of metal-type and electron energy can be explained.

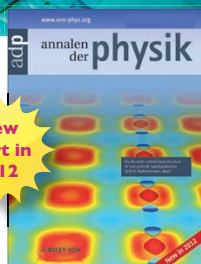
THU 52**Electrically Tunable Band Gap in Silicene**

Viktor Zólyomi¹, Neil D. Drummond¹, Vladimir I. Fal'ko¹

¹Department of Physics, Lancaster University, Lancaster

We report calculations of the electronic structure of silicene and the stability of its weakly buckled honeycomb lattice in an external electric field oriented perpendicular to the monolayer of Si atoms. We find that the electric field produces a tunable band gap in the Dirac-type electronic spectrum, the gap being suppressed by a factor of about eight by the high polarizability of the system. At low electric fields, the interplay between this tunable band gap, which is specific to electrons on a honeycomb lattice, and the Kane-Mele spin-orbit coupling induces a transition from a topological to a band insulator, whereas at much higher electric fields silicene becomes a semimetal.

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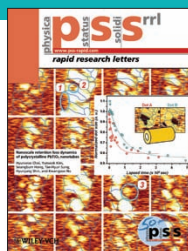
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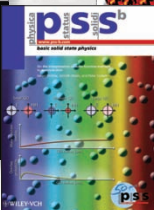
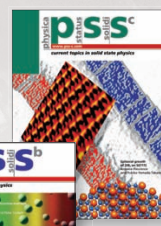
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Non-carbon materials; NEMS, doping of graphene

Friday, March 9th

- 08:30 – 09:00 **A. Kis, Lausanne**
Single layer MoS₂: devices, electronics and mechanics
- 09:00 – 09:30 **D. Mihailovic, Ljubljana**
Collective phenomena in real time and low temperature in low-dimensional transition metal chalcogenides
- 09:30 – 10:00 **A. Schliwa, Berlin**
How the crystallographic symmetry influences the electronic properties of quantum dots
- 10:00 – 10:30 **Coffee break**
- 10:30 – 11:00 **A. Bachtold, Barcelona**
Electromechanical resonators made from nanotubes and graphene
- 11:00 – 11:30 **S. Bunch, Boulder**
Ultrastrong Adhesion and other Graphene Mechanical Wonders
- 11:30 – 12:00 **V. Pereira, Singapore**
Strain, wrinkles and other aspects of the thinnest crystalline membrane
- 12:00 – 17:00 **Mini-Workshops**
- 17:00 – 17:30 **D. Haberer-Gehrmann, Dresden**
Electron-Phonon Interactions in quasi-free-standing Graphene
- 17:30 – 18:00 **V. Krstic, Dublin**
Superstructuring of graphene: charge-transport in superlattices
- 18:00 – 18:30 **A. Jorio, Belo Horizonte**
Summary
- 18:30 – 20:00 **Break**
- 20:00 **Bauernbuffet – Farewell**

Friday, March 9th

Non-carbon materials; NEMS, doping of graphene

08:30**Single layer MoS2: devices, electronics and mechanics**Andras Kis¹¹EPFL, Lausanne

After quantum dots, nanotubes and nanowires, two-dimensional materials in the shape of sheets with atomic-scale thickness represent the newest addition to the diverse family of nanoscale materials. I will show here our work on single layer MoS2, a direct-gap semiconductor. We have exfoliated single layers 6.5 Angstrom thick from bulk crystals of semiconducting MoS2, using the micromechanical cleavage technique commonly used for the production of graphene. Our nanolayers are mechanically and chemically stable under ambient conditions. We have fabricated transistors based on single-layer MoS2 which demonstrate that this material has several advantages over silicon for potential applications in electronics and that it has the capability to amplify signals and perform logic operations. Finally, I will show our work on suspended MoS2 membranes that show ripples similar to those observed in graphene. MoS2 also has superior mechanical properties: higher stiffness than steel and breaking strength at the theoretical limit which makes it suitable for integration in flexible electronics.

09:00**Collective phenomena in real time and low temperature in low-dimensional transition metal chalcogenides**Dragan Mihailovic¹¹Jozef Stefan Institute, Ljubljana

An exciting feature of low-dimensional transition metal chalcogenide (TMC) systems is that they display a variety of collective phenomena which are not commonly seen in carbon systems. For example, both quasi-2D and 1D materials display a variety of charge-ordering transitions and interplay with superconductivity. In this presentation I will show coherent charge ordering system trajectories in 2D chalcogenides leading to the formation of multilayer domain structures within a 20 nm layer on the femtosecond timescale (1). Under some circumstances these topological defects may become metastable. The manifestation of collective behaviour in 1D chalcogenide systems as Luttinger liquids is quite unmistakable, leading to very peculiar form of giant paramagnetism upon modification by doping, which - in spite of the huge susceptibility and Stoner enhancement factor - do not undergo the expected collective transition to an antiferromagnetic state.

The work was done with T.Mertelj, R.Yusupov, P.Kusar, V.Kabanov, S.Brazovski, J.Strle, M.Strojnjk, P.Topolovsek, C.Gadermaier, V.Nicolosi and A.Omerzu.

1. R.Yusupov et al. Nat. Phys.6, 681 (2010)

09:30

How the crystallographic symmetry influences the electronic properties of quantum dots

Andrei Schliwa¹, Axel Hoffmann¹, Christian Thomsen¹

¹Institut für Festkörperphysik, TU-Berlin

Quantum dots are well known for their atomic-like properties, which can be tailored to meet a wide range of application specific target properties. Epitaxial- as well as colloidal QDs are produced in zinc-blende- (zb) as well as in wurtzite (wz) type crystallographic phase. Hence, it is of high importance to understand the impact of the underlying crystallographic symmetry on the quantum dots electronic properties. This interrelation will be discussed using the examples of epitaxial InAs/GaAs (zb) and GaN/AlN (wz) QDs as well as colloidal CdSe/CdS (zb/wz) QDs. Special emphasis is put on the Coulomb interaction and exciton-phonon interaction.

Friday, March 9th

Non-carbon materials; NEMS, doping of graphene

10:30

Electromechanical resonators made from nanotubes and graphene

Adrian Bachtold¹

¹ICN Barcelona

Carbon nanotubes and graphene offer unique scientific and technological opportunities as nanoelectromechanical systems (NEMS). Namely, they have allowed the fabrication of mechanical resonators that can be operable at ultra-high frequencies and that can be employed as ultra-sensitive sensors of mass or charge. In addition, nanotubes and graphene have exceptional electron transport properties, including ballistic conduction over long distances. Coupling the mechanical motion to electron transport in these remarkable materials is thus highly appealing. In this talk, I will review some of our recent results on nanotube and graphene NEMSs, including the nonlinear nature of damping in these resonators, and mass sensing at the proton mass level.

11:00

Ultrastrong Adhesion and other Graphene Mechanical Wonders

J. Scott Bunch¹

¹Department of Mechanical Engineering, University of Colorado, Boulder, Colorado

Graphene, a single layer of graphite, represents the first truly two dimensional atomic crystal. It consists solely of carbon atoms covalently bonded in a hexagonal chicken wire lattice. This unique atomic structure gives it remarkable electrical, mechanical, and thermal properties. It has the highest electrical and thermal conductivity among all materials known. However, it is the mechanical properties of this wonder material that fascinate our group the most. It is the thinnest, stiffest, and strongest material in the world as well as being impermeable to all standard gases. In this talk, I will review some of our recent experimental results on ultrastrong adhesion of graphene and the mechanical properties of a new class of ultrathin oxide membranes.

11:30**Strain, wrinkles and other aspects of the thinnest crystalline membrane**Vitor M Pereira¹¹Department of Physics, National University of Singapore, Singapore

Graphene is the thinnest crystal in the universe, and the only metallic membrane whose structure can be simulated accurately at the atomistic level.

The 2D nature makes it sensitive to strain in ways that can be explored much beyond what is allowed in conventional electronic systems. This lead to the development of the concept of strain-engineered graphene, whereby strain is seen as a means to influence essentially all its intrinsic properties, ranging from the electronic structure, to transport, chemical activity, optical absorption, or correlations.

I briefly review the current status of the effort towards strain-engineered graphene, and shall describe in more detail how ubiquitous wrinkles might affect the motion of the Dirac electrons in graphene.

Wrinkling in 2D membranes is intimately associated with the presence of geometrical singularities which arise from the necessity of the system to relieve as much in-plane stain as possible. Such singular structures directly couple to electrons via local strain and curvature modulations that can strongly modify the local electronic structure and impact the conductivity due to enhanced scattering by strongly confining potentials.

17:00**Electron-Phonon Interactions in quasi-free-standing Graphene**Danny Haberer-Gehrmann¹¹Institute for Solid State Research, Leibniz IFW Dresden, Dresden

Despite the intense investigation of electron-phonon interactions in electron doped graphite intercalation compounds (GICs), there are still several open topics regarding coupling strength, mechanism for superconductivity as well as the anisotropy of the coupling constant in momentum space. Employing high quality quasi-free-standing graphene and measuring its spectral function, we are able to investigate the electron-phonon coupling in a long range ordered sample for several dopants. Our results therefore allow a conclusive determination of the angle dependent Eliashberg function (phonon density of states times the squared electron-phonon matrix elements), which is the central quantity of a coupled electron-phonon system. Furthermore, we shine new light on the long-standing problem of the asymmetry in the electron-phonon coupling constants in the 2D Brillouin zone of graphene. Finally, we discuss the effects of various alkali metal dopants and relationships to the corresponding GICs.

17:30**Superstructuring of graphene: charge-transport in superlattices**Vojislav Krstić¹¹Trinity College Dublin, Dublin

Being an all-surface material, the transport properties of graphene are altered by a wide range of interactions with the environment. These interactions can originate from molecular and atomic species adsorbed from the atmosphere on the graphene or from the presence of a specific substrate surface. Such interactions can lead to an unintentional doping but most importantly introduce a variety of charge-carrier scattering centres such as charged impurities, lattice-strain or resonant scatterers. Another common feature is the circumstance that all these scattering centres are randomly distributed all over the graphene and thus represent a disordered, non-coherent scatterer field.

The introduction of a specific symmetry to a scatterer field represents a qualitative change in the (overall) scattering of a charge-carrier. Moreover, graphene charge-carriers behave as mass-less Dirac-particles, and scattering from scattering centres differs from the case of mass-carrying fermions. Such a situation is achieved by imposing a superlattice of scattering centres on graphene. In the present work the impact of a superlattice on the charge-transport properties in graphene-devices is discussed.

18:00**Summary**AdoJorio¹¹Belo Horizonte, Brazil

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