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International Winterschool on Electronic Properties of Novel Materials
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 23rd International Winterschool on:
Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of twenty-two 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 Müller	accomodation, sponsoring
Nils Rosenkranz	registration, finance
Marcel Mohr	video transfer and recording, internet
Hagen Telg	general assistance
Harald Scheel	receipts, technical assistance
Dirk Heinrich	technical assistance
Norman Tschirner	computer, internet, e-payment

Also the managers of the hotel, Frau Mayer and her son Herr Mayer, and their staff promised to help us wherever they can. We want to acknowledge their help and also that of Sabine Morgner in the organization of the IWEPNM 2009.

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, Peter, Hans, and Siegmar

Chairmen

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P. Dinse (Darmstadt)
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D. Zhu (CN)

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 • 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 2009 starts on Saturday, 7 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 14 March, breakfast. There will be a reception party on 7 March, after dinner, and a farewell party including dinner on Friday, 13 March.

Transport

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

Addresses

The address of the Winterschool is:
IWEPNM 2009, Hotel Sonnalp, A–6365 Kirchberg/Tirol, Austria
Tel: ++43 5357 27410, Fax: ++43 5357 2741 200
e-mail: info@hotelsonnalp.info, Web: www.tiscover.at/sonnalp.parkhotel
All questions concerning the IWEPNM 2009 should be directed to:
Prof. 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 2009 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.

During the conference

If you want 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.

Proceedings

The contributions to the IWEPNM 2009 will be published in physica status solidi. The expected date for the appearance of the proceedings is September 2009. **Contributions can only be published if they arrive before the 30 April. Online submission** will be used, which you can find under the following address: http://conferences.wiley-vch.de/v3. 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

Make sure to refer to the current version of the instructions for authors:
http://www3.interscience.wiley.com/cgi-bin/jabout/40000761/instructions.html
In particular, the following requirements should be met:

- Your manuscript should be written using our Word

  http://www.wiley-vch.de/vch/journals/2231/public/pss_abc_2008_word.zip

  or LaTeX

  http://www.wiley-vch.de/vch/journals/2231/public/pss_abc_2008_latex.zip

  template.
- Relevant PACS numbers (a maximum of six codes) must be given, see the full and most recent classification system (PACS 2008) at http://www.aip.org/pacs. Always use the complete form, such as 32.50.+i, 71.70.Ej. The page limit for invited oral talks is 6 for poster contributions 4 pages. Submission deadline is April 30, 2009.

Manuscript submission

For online submission please go to http://conferences.wiley-vch.de/v3. Your login details will be emailed to you by the conference organizers in due time. Select PHYSICA STATUS SOLIDI as the journal and choose IWEPNM 2009 from the list of projects. Once you there, click on “Create manuscript” on the left side of the screen and follow the instructions.

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.
Example: smith_version2.doc. Please note that after submitting a manuscript, you can no longer modify it.

IWEPNM 2009
CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 8.03.	morning	Mehring
	morning, after coffee break	Loiseau
	evening	Pichler
Monday, 9.03.	morning	Kuzmany
	morning, after coffee break	Saito, R.
	evening	Kaiser, A.
Tuesday, 10.03.	morning	Novoselov
	morning, after coffee break	Maruyama
	evening	Obraztsova
Wednesday, 11.03.	morning	Mauri
	morning, after coffee break	Kürti
	evening	Hartschuh
Thursday, 12.03.	morning	Robertson
	morning, after coffee break	Roth
	evening	Forro
Friday, 13.03.	morning	Bockrath
	morning, after coffee break	Dinse
	evening	Kamaras

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 8 March	Monday 9 March	Tuesday 10 March	Wednesday 11 March	Thursday 12 March	Friday 13 March
Topics	**Synthesis and selection of carbon nanotubes**	**Graphene I and quantum dots**	**Graphene II and theory of carbon nanotubes**	**Optics of carbon nanotubes**	**Applications of carbon nanotubes**	**Transport and magnetic properties of carbon nanotubes**
8:30	High efficiency metal-semiconductor separation of SWNTs by using agarose gel KATAURA	Spin injection, transport and manipulation in graphene field effect transistors. VAN WEES	Graphene mechanics, tribology, Raman spectra under strain, and NEMS HONE	Understanding environmental effects on the electronic and vibrational excitations and dynamics in carbon nanotubes PEREBEINOS	Nanotube applications: from fascinating dreams to increasingly the marketplace BAUGHMAN	Highly efficient electron-hole pair generation via impact ionization in CNT p-n junction photodiodes GABOR
9:00	In situ electron microscopy observations on CNTs and related structures during deformations, growth and transformations JIN		Doping effects in pristine and epitaxial graphene KERN			Nuclear spins in nanostructures LOSS
9:30	Electronic properties of pristine and doped carbon nanotubes SAITO, S.	Graphene: the magic of flat carbon NOVOSELOV	Microscopic studies of graphene MEYER	Exciton states and phonon softening phenomena in SWCNTs SAITO, R.	Progress toward negative index lenses CARROLL	Pumping single electrons with SWNT SIEGLE
10:00	Coffee break					
10:30	Preparation, characterization, and application of monodisperse single- and double-walled CNTs HERSAM	Graphene and graphene superlattices: pseudospin, electron-electron and electron-phonon effects LOUIE	Optical spectroscopy of single and few-layer graphene HEINZ	Near-field optical investigations of individual single-walled carbon nanotubes HARTSCHUH	Sparse random arrays of pristine and doped carbon nanotubes: A tuneable meta material KRAMBERGER	Electrically detected coherent spin control in carbon based semiconductors BÖHME
11:00	Separating SWNTs by length, electronic property and chiral index KAPPES	Electron-phonon coupling in graphene ATTACALITE	Scanning tunneling spectroscopy and transport measurements in suspended graphene ANDREI	Characterization of isolated metallic and semiconducting nanotubes by Raman spectroscopy TELG	In vitro effects of carbon based materials BRUINICK	Electron spin resonance of Luttinger liquids and single-wall carbon nanotubes DORA
11:30	Low-voltage high resolution TEM of carbon nanomaterials WARNER	Stability, chemical structure, and Clar's aromatic sextets of hydrogen-terminated graphene ribbons MAURI	Raman spectroscopy of graphene under uniaxial strain FERRARI	Disorder in sp^2 nanocarbons: doping, ion bombardment and substrat interaction JORIO	Doping strategy of carbon nanotubes LEE, Y.H.	Doping of single-walled carbon nanotubes with phosphorous atoms KRSTIC

12:00-17:00	Mini worksshops					
17:00 - 18:30	Dinner					**17:00** Bile-salt solubilization offers high resolution and selectivity for the spectroscopy of SWCNTs GOOVAERTS
18:30	Excitement of nano-test tube chemistry inside SWCNTs SHIOZAWA	Probing diffusive and ballistic transport in graphene FUHRER	Classification and diffraction of quasi one-dimensional crystals DAMNJANOVIC	Spectral features due to dark exciton in photoluminescence map of SWCNTs MARUYAMA	Advances in the chemistry and applications of carbon nanomaterials HADDON	
19:00	Carbon nanomaterials for advanced applications SCHARFF	Graphene quantum dots STAMPFER	NaPhoD – nano-hybrids for photonic devices AMBROSCH-DRAXL	Linear optical spectra and relaxation dynamics in SWCNTs MALIC	Synthesis and characterisation of ultra-thin conducting carbon films DUESBERG	**17:30** Two-phonon Raman spectroscopy of one-, two-layered graphene and CNTs OBRAZTSOVA
19:30	CNT-polymer composites for possible thermoelectric energy converting materials PARK	Molecular states of correlated electrons in quantum dots RONTANI	Electrodynamics of carbon nanotubes: principles, device applications and open questions MAKSIMENKO	Optical spectroscopy of individual single-walled carbon nanotubes LOUNIS	Sensing mechanism behind the metal-decorated SWNT-FETs LEE, J.O.	**18:00** IWEPNM09 - Conference summary HEINZ **18:30 - 20:00** Break
20:00	Supramolecular nanostructures of a phthalocyanine-C60 fullerene conjugate TORRES	Poster I Monday	Poster II Tuesday	Resonant Raman of 0.3nm single-walled carbon nanotubes TANG	Poster III Thursday	Bauernbuffet Farewell
20:30						
Topics	Synthesis and selection of carbon nanotubes	Graphene I and quantum dots	Graphene II and theory of carbon nanotubes	Optics of carbon nanotubes	Applications of carbon nanotubes	Transport and magnetic properties of carbon nanotubes
	Sunday 8 March	Monday 9 March	Tuesday 10 March	Wednesday 11 March	Thursday 12 March	Friday 13 March

PROGRAM

AND

ABSTRACTS


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Synthesis and selection of carbon nanotubes

8:30 – 9:00	H. Kataura, JP *High efficiency metal-semiconductor separation of single-wall carbon nanotubes by using agarose gel*
9:00 – 9:30	C. Jin, JP *In situ electron microscopy observations on CNT and related structures during deformations, growth and transformations*

9:30 – 10:00	S. Saito, JP *Electronic properties of pristine and doped carbon nanotubes*

10:00 – 10:30	Coffee break

10:30 – 11:00	M. C. Hersam, US *Preparation, characterization, and application of monodisperse single-walled and double-walled carbon nanotubes*
11:00 – 11:30	M. M. Kappes, DE *Separating SWNTs by length, electronic property and chiral index*
11:30 – 12:00	J. H. Warner, UK *Low-voltage high resolution TEM of carbon nanomaterials*

12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner

18:30 – 19:00	H. Shiozawa, UK *Excitement of nano-test tube chemistry inside SWNTs*
19:00 – 19:30	P. Scharff, DE *Carbon nanomaterials for advanced applications*
19:30 – 20:00	Y. W. Park, KR *CNT-polymer composites for possible thermoelectric energy converting materials*
20:00 – 20:30	T. Torres, ES *Supramolecular nanostructures of a phthalocyanine C60 fullerene conjugate*

Sunday, March 8

8:30
High efficiency metal-semiconductor separation of single-wall carbon nanotubes by using agarose gel

H. Kataura[1] T. Tanaka[1] Y. Miyata[1] S. Fujii[1] D. Nishide[1] K. Yanagi[1] Y. Feng[2] K. Matsuishi[2] Y. Maniwa[3]
[1]JST, CREST, Nanotechnology Research Institute, AIST, Tsukuba, Japan
[2]Institute of Materials Science, University of Tsukuba, Tsukuba, Japan
[3]Department of Physics, Tokyo Metropolitan University, Tokyo, Japan

Metal-semiconductor separation is indispensable for practical applications of single-wall carbon nanotubes (SWCNTs), such as thin film transistors and transparent conducting films. After the great works by Arnold et al.[1], now we can obtain high-purity metallic and semiconducting SWCNTs by using density gradient ultracentrifugation. For the industrial application, however, we still have to reduce the time and cost of the separation. Recently, we found the agarose gel can separate SWCNTs-SDS solution into metallic and semiconducting phases without any special treatment[2]. This new method can separate SWCNTs with high purity, high efficiency, and totally low cost. In this presentation, we will show our recent progress in the separation and some device applications.

1. M.S. Arnold et al., Nat. Nanotechnol. 1 (2006) 60.
2. T. Tanaka et al., Appl. Phys. Express 1 (2008) 114001.

9:00
In situ electron microscopy observations on carbon nanotubes and related structures during deformations, growth and transformations

Chuanhong Jin[1] Kazu Suenaga[1] Sumio Iijima[1]
[1]Nanotube Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Investigating the physical and chemical properties of individual quantum objects has long been endeavored with the precise atomic configurations. Although the measurements of the transport and electronic properties of carbon nanotubes were previously performed in TEM, the real atomic resolution was not achieved in these experiments. In situ HR-TEM studies with a higher spatial resolution have been just made possible by the development of more stable specimen holder (Nanofactory) and the advancement of the electron optics in TEM based on the aberration correctors (CEOS). We will present here some examples of the in situ HR-TEM studies of carbon nanotubes: joining and growth behavior, migrations of the individual atomic defects (vacancies) at the elevated temperatures, catalytic growth of fullerenes, as well as formation of lip-lip networks.

The work presented here was partially supported by the CREST and the KAKENHI. Fellowships of the JSPS and the Balzan Foundation (through Meijo Univ) are also acknowledged.

9:30

Electronic properties of pristine and doped carbon nanotubes

Susumu Saito
Department of Physics, Tokyo Institute of Technology, Tokyo

Doping into semiconductor carbon nanotubes is of high interest from the viewpoint of their application as nanodevice materials as well as from the viewpoint of superconductivity with high transition temperatures to be realized in covalent-bond based materials with light elements. We study the electronic structure as well as the energetics of substitutionally B-doped carbon nanotubes in the framework of the density-functional theory. Results are discussed with emphasis on the importance of electron correlation which is pointed out to be of crucial importance in predicting so-called impurity levels in semiconductors in general. In addition to these doped carbon nanotubes, we report electronic properties of various thincarbon nanotubes including armchair and chiral nanotubes. Details of the electronic structure of thin nanotubes are highly important at present since the experimental purification of thin nanotubes is in progress in several groups. We point out that the geometry optimization turns out to be very important in predicting the electronic properties of thin carbon nanotubes.

10:30

Preparation, characterization, and application of monodisperse single-walled and double-walled carbon nanotubes

Mark C. Hersam
Department of Materials Science and Engineering and Department of Chemistry, Northwestern University, Evanston, IL 60208-3108, USA

Large-scale production of high purity carbon nanotubes has the potential to enable or improve many applications. Recently, we have developed a scalable and flexible technique for sorting single-walled carbon nanotubes (SWNTs) by their physical and electronic structure using density gradient ultracentrifugation (DGU). Diameter-sorted metallic SWNTs yield semi-transparent conductive films with tunable optical absorption. On the other hand, semiconducting SWNTs enable thin film transistors with high switching ratios and drive currents. Most recently, chiral surfactants have been utilized for DGU-based sorting of SWNT enantiomers. In all cases, analytical ultracentrifugation measurements allow the SWNT surfactant loading to be quantified and optimized for improved DGU sorting. This talk will also delineate DGU sorting of double-walled carbon nanotubes (DWNTs). Since DWNTs possess a buoyant density that is intermediate between SWNTs and multi-walled carbon nanotubes, a two-step DGU process has been developed for high purity DWNTs. DGU-sorted DWNTs enable characterization of the fundamental properties of DWNTs and yield high performance transparent conductive films.

11:00
Separating SWNTs by length, electronic property and chiral index

Manfred M. Kappes[1] Frank Hennrich[1] Sergei Lebedkin[1] Ninette Stürzl[1] Oliver Kiowski[1]
[1]Institut für Physikalische Chemie, Universität Karlsruhe and Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany

Density gradient ultracentrifugation, electrophoresis and selective dispersion have been used (sometimes in combination) to fractionate SWNTs according to length, electronic property and chiral index. The talk will address various associated mechanistic issues and will present spectroscopic measurements on resulting fractionated samples.

11:30
Low-voltage high resolution TEM of carbon nanomaterials

Jamie H Warner[1] Mark H. Rümmeli[2] Yasuhiro Ito[1] Bernd Büchner[2] Hisanori Shinohara[3] G. Andrew D. Briggs[1]
[1]Department of Materials, University of Oxford, UK
[2]IFW Dresden, Germany
[3]Department of Chemistry, Nagoya University, Japan

The emergence of aberration-corrected low-voltage high resolution transmission electron microscopy opens many new exciting possibilities for examining the atomic structure of carbon nanomaterials. This enables the determination of the chirality of nanotubes, the orientation and edge termination of graphene sheets and their packing arrangement. Accelerating voltages of 80 kV lead to significant reduction in the knock-on damage to sp2 carbon atoms in graphene based nanomaterials such as fullerenes, nanotubes and graphene. I will present our latest findings that shed light on how electrons accelerated at 80 kV interact with carbon atoms and the new forms of damage that occur. We find 80 kV electron beam irradiation can lead to unique structural transformations that are not always detrimental. We track the evolution in real time with spatial resolution on the angstrom scale and temporal resolution down to 80 milliseconds. Our results involve examining graphene and few layer graphene sheets, SWNTs and DWNTs, and peapods (i.e fullerenes/metallofullerenes inside SWNTs).

18:30

Excitement of nano-test tube chemistry inside single-walled carbon nanotubes

Hidetsugu Shiozawa[1] S. Ravi P. Silva[1] Zheng Liu[2] Kazu Suenaga[2] Hiromichi Kataura[2] David Batchelor[3] Christian Kramberger[4] Thomas Pichler[4]
[1]Advanced Technology Institute, University of Surrey, UK
[2]AIST, Japan
[3]Bessy II, Germany
[4]Faculty of Physics, University of Vienna, Austria

The excitement of nano-test tube chemistry in single-walled carbon nanotubes is exemplified in our study on the growth of inner tubes from encapsulated molecules. Using different oragnometallic precursors we study the mechanism for the catalytic growth of carbon nanotubes. The structural and chemical status of encapsulated elements is identified from Raman, photoemission, core-level absorption spectroscopy and transmission electron microscopy. Electron doping through the 1D van Hove singularity of single-walled carbon nanotubes is obtained by using an organocerium compound as a precursor filling. From a resonance photoemission study we show that increased doping of the filled tubes greatly enhances the density of conduction electrons. Through electronic excitations from the carbon 1s core level to the 1D van Hove singularity of initial semiconducting tubes, we demonstrate that their increased density of conduction states leads to enhanced screening of the photo-excited core hole potential. This fact illustrates the importance of many body effects in understanding core level excitation process in carbon nanotubes.

19:00

Carbon nanomaterials for advanced applications

Peter Scharff[1] Uwe Ritter[1] Svetlana Prylutska[2]
[1]Chemie, Elektrochemie und Galvanotechnik, Ilmenau, Germany
[2]Kyiv National Shevchenko University, Kyiv, Ukraine

Discrete spherical carbon molecules offered a broad variety of possible reactions to the chemists, whereas the nanotubes stand out because of their unique physical properties. Exemplarily some new applications of carbon nanomaterials are demonstrated and the research focus in Ilmenau on these materials will be demonstrated. Chemically functionalized MWCNT arrays can work as ultra sensitive sensors for the detecting of chemical substances, for the detection of reactive gas molecules or specific biological targets. Charge transfer or small changes in the charge-environment of a nanotube can cause drastic changes to its electrical properties. The aim is using these nanomaterials as an electrical probe of chemical and biological interaction. Carbon nanotubes can be exited by light in the same way as fullerenes and the exiting energy can be transferred to other molecules with high efficiency, which is used in biological and medical applications. The biological effects of fullerene derivatives will be demonstrated by the generation of reactive oxygen species. The obtained experimental data allow us to consider these fullerene materials as potential agents for a photodynamic therapy.

19:30

CNT-polymer composites for possible thermoelectric energy converting materials

Yung Woo Park[1] Siegmar Roth[2]
[1]Department of Physics and Astronomy, Seoul National University, Seoul
[2]SYNEUROPE, Stuttgart, Germany

Thermoelectric power is a zero current transport coefficient defined as $S = \Delta V/\Delta T$. By applying temperature gradient to the system, electricity is generated. An energy converting device from thermal energy to electricity can be developed using the thermoelectricity. The figure of merit $ZT = TS2\sigma/\kappa$ is a measure of the efficiency of the thermoelectric energy convergence. Therefore, finding materials of high electrical conductivity (σ), high thermoelectric power (S) and low thermal conductivity (κ) is the key issue for highly efficient thermoelectric energy converting devices. CNT shows high room temperature thermoelectric power value $SRT \approx +100\mu V/K$ with metallic conductivity and it can be doped to n- or p-type semiconductors with relatively high room temperature thermoelectric power values. Although the thermal conductivity of CNT is high, it can be reduced by mixing the CNT with appropriate polymers. Therefore, we propose the CNT-polymer composites as possible high figure of merit materials for the thermoelectric energy converting devices.

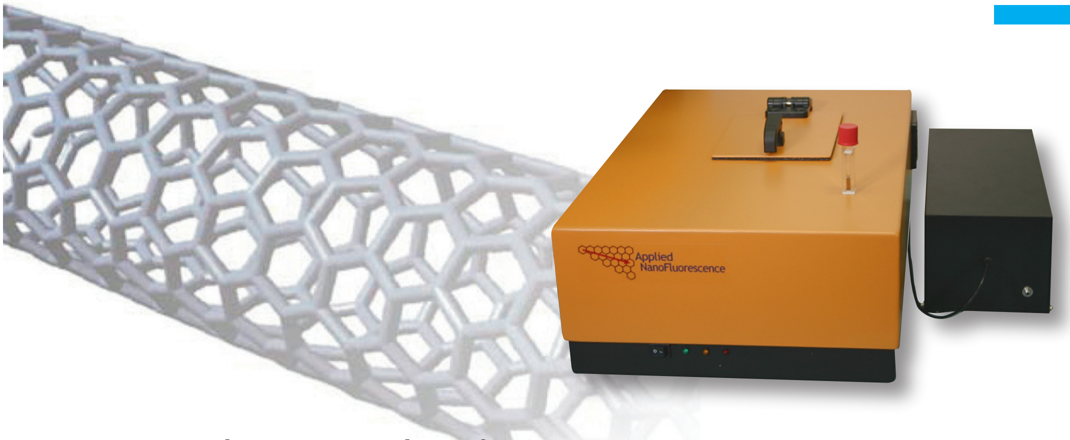
20:00

Supramolecular nanostructures of a phthalocyanine-C60 fullerene conjugate

Tomas Torres[1] Giovanni Bottari[1]
[1]Organic Chemistry C-I, Autonoma University of Madrid, Madrid

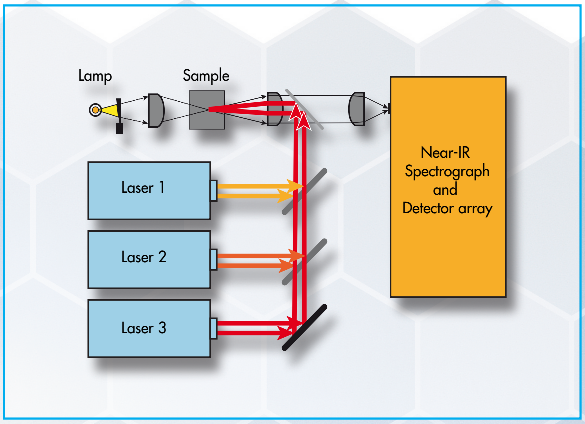
The construction of highlyâordered supramolecular architectures in which organic mole- cules are organized on surfaces across multiple length scales represents a keyâissue within the fastâgrowing field of supramolecular electronics. One of the most promising methods for the construction of these supramolecular assemblies relies on the selfâorganization ability of piâconjugated systems. Phthalocyanines (Pcs) are planar, two-dimensional (2-D) aromatic molecules able to self-assemble into stacks through pi-pi supramolecular interactions. These macrocycles possess outstanding electrical and optical properties. Up to date a few molecular and supramolecular architectures incorporating a Pc macrocycle and a C60 fullerene moiety (i.e. a Pc-C60 dyad) have been prepared and studied. In this communication we report on a covalently-linked Pc-C60 fullerene conjugate which is able to self-organize on graphite forming fibers and films as revealed by atomic force microscopy (AFM) studies. These nanostructures, which possess outstanding nanoscale electrical conductivity, has been also organised on SWNT.

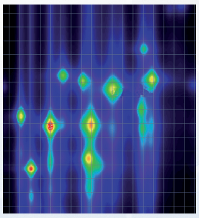
The NS1 Nanospectralyzer

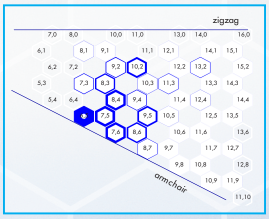


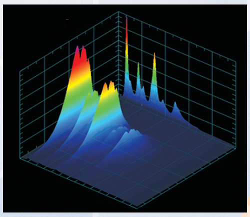
Automatic Fluorimetric Analysis of SWNTs

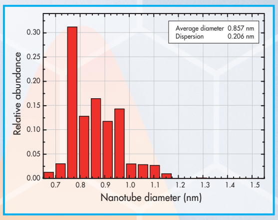
- Rapid near-IR-fluorescence and absorption Spectroscopy
- Trace detection capability
- Three lasers, compact design
- Small sample volumes
- Sophisiticated versatile software
- Automatic display of (*n*, *m*) distributions in seconds
- Turn-key system operation
- Support from pioneering nanotube spectroscopists
- Generous software updates reflect new research findings











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Graphene I and quantum dots

8:30 – 9:30	B. v. Wees, NL *Spin injection, transport and manipulation in graphene field effect transistors.*
9:30 – 10:00	Novoselov, UK *Graphene: the magic of flat carbon*
10:00 – 10:30	Coffee break
10:30 – 11:00	S. G. Louie, US *Graphene and graphene superlattices: pseudospin, electron-electron and electron-phonon effects*
11:00 – 11:30	C. Attaccalite, ES *Electron-phonon coupling in graphene*
11:30 – 12:00	F. Mauri, FR *Stability, chemical structure, and Clar's aromatic sextets of hydrogen-terminated graphene ribbons*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	M. S. Fuhrer, US *Probing diffusive and ballistic transport in graphene*
19:00 – 19:30	C. Stampfer, CH *Graphene quantum dots*
19:30 – 20:00	M. Rontani, IT *Molecular states of correlated electrons in quantum dots*
20:00 – 21:00	Poster Session I – MON

Monday, March 9

8:30

Spin injection, transport and manipulation in graphene field effect transistors.

Bart van Wees
Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

I will give an overview of our experiments on single graphene layer field effect devices with ferromagnetic contacts. The use of the so-called non-local geometry allowed a detailed investigation of various aspects of spin injection, spin transport and spin manipulation.

We found that: a) Spins can be injected into graphene with an injection efficiency up to 35 percent [1]. b) Spins can be transported through the graphene with a spin relaxation length of about 1.5 micrometer. By applying a perpendicular magnetic field Hanle spin precession could be studied [2]. c) By applying a large DC electric field the transport of spins between injector and detector could be facilitated using carrier drift [3]. d) The spin relaxation was found to be slightly anisotropic, with spins perpendicular to the graphene plane relaxing faster than spins in the plane [4]. The potential of graphene for future spintronics applications will be discussed.

[1] C. Jozsa et al., Phys. Rev. B Rap. Com. to be published,(cond-mat 0811-2960) [2] N. Tombros et al, Nature 448, 571 (2007) [3] C. Jozsa et al., Phys. Rev. Lett. 100, 236603 (2008) [4] N. Tombros et al., Phys. Rev. Lett. 101, 046601 (2008)

9:30

Graphene: the magic of flat carbon

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School of Physics & Astronomy, University of Manchester, Manchester, UK

When one writes by a pencil, thin flakes of graphite are left on a surface. Some of them are only one angstrom thick and can be viewed as individual atomic planes cleaved away from the bulk. This strictly two dimensional material called graphene was presumed not to exist in the free state and remained undiscovered until the last year. In fact, there exists a whole class of such two-dimensional crystals. The most amazing things about graphene probably is that its electrons move with little scattering over huge (submicron) distances as if they were completely insensitive to the environment only a couple of angstroms away. Moreover, whereas electronic properties of other materials are commonly described by quasiparticles that obey the Schrödinger equation, electron transport in graphene is different: It is governed by the Dirac equation so that charge carriers in graphene mimic relativistic particles with zero rest mass. The very unusual electronic properties of this material as well as the possibility for itâs chemical modification make graphene a promising candidate for future electronic applications.

10:30

Graphene and graphene superlattices: pseudospin, electron-electron and electron-phonon effects

Steven G. Louie
Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory

I discuss some recent theoretical results we obtained on the electronic and optical properties of graphene and graphene superlattices. The low-energy excitations in these carbon nanostructures, which are 2D massless Dirac fermions, exhibit a number of unexpected behaviors. We showed that, owing to the chiral nature (pseudospin) of the electronic states, the carrier dynamics in graphene exhibits anomalous anisotropy when subjected to an external periodic potential of nanometer dimensions (called graphene superlattices). Under appropriate conditions, these graphene superlattices are predicted to be electron supercollimators and new generation of massless Dirac fermions may be created. Our first-principles calculations revealed that electron-electron and electron-phonon interactions give rise to significant corrections to the quasiparticle band velocity of graphene and that both are central to the understanding of the electron linewidths as measured in angle-resolved photoemission experiment. We also investigated the optical properties of single- and bi-layer graphene with many-electron effects included. Although these systems are semimetals, excitonic effects are found to be quite significant in their optical absorption spectrum.

11:00

Electron-phonon coupling in graphene

Claudio Attaccalite
Unidad de Fisica de Materiales, Universidad del Pais Vasco, San Sebastian

We studied the effect of electron-electron correlation on the full three dimensional dispersion of the π-bands, Fermi velocities and effective masses of graphite/graphene. The results are then compared with recent experiments obtained by angle resolved photo-emission spectroscopy, and we found that the band structure obtained by density-functional theory (in LDA approximation) strongly underestimates the slope of the bands.Successively we investigate the effect of electronic correlation on the electron-phonon coupling (EPC) using different approximations, ranging from Hartree-Fock to GW. We found that GW renormalize the EPC at the A'1 **K** mode by almost 80% with respect to density functional theory in LDA approximation. The obtained phonon slope of the A'1 **K** is almost two time larger than the LDA one, in agreement with phonon dispersions from inelastic x-ray scattering and Raman spectroscopy experiments.

11:30

Stability, chemical structure, and Clar’s aromatic sextets of hydrogen-terminated graphene ribbons

Francesco Mauri[1] Tobias Wassmann[1] Ari P. Seitsonen[1] A. Marco Saitta[1] M. Lazzeri[1]
[1]IMPMC, Universite Pierre et Marie Curie - Paris 6, Paris

We determine the stability, the geometry, the electronic, and magnetic structure of hydrogen-terminated graphene-nanoribbon edges as a function of the hydrogen content of the environment by means of density functional theory [1]. Antiferromagnetic zigzag ribbons are stable only at extremely low ultravacuum pressures. Under more standard conditions, the most stable structures are the mono- and dihydrogenated armchair edges and a zigzag edge reconstruction with one di- and two monohydrogenated sites. At high hydrogen concentration âbulkâ graphene is not stable and spontaneously breaks to form ribbons, in analogy to the spontaneous breaking of graphene into small-width nanoribbons observed experimentally in solution. The stability and the existence of exotic edge electronic states and/or magnetism is rationalized in terms of Clarâs aromatic sextets.

[1] T. Wassmann, A.P. Seitsonen, A.M. Saitta, M. Lazzeri, and F. Mauri, Phys. Rev. Lett. 101, 096402 (2008)

18:30

Probing diffusive and ballistic transport in graphene

Michael S. Fuhrer
Department of Physics, University of Maryland, College park

I will discuss experiments performed on atomically-clean[1] graphene on SiO_2 in ultra-high vacuum to determine the electron scattering rates from charged impurities[2], point defects[3], and phonons (graphene acoustic phonons and substrate polar optical phonons)[4]. The experiments point out both the promise of graphene as well as the technological challenges that lie ahead in realizing better samples. I will also discuss briefly experiments in the ballistic transport limit in few-100 nm single-layer (bi-layer) graphene samples, in which charge transport is dominated by resonant transmission of massless (massive) particle-in-a-box like states confined between the source and drain electrodes[5].

[1] M. Ishigami, J. H. Chen, W. G. Cullen, M. S. Fuhrer, and E. D. Williams, Nano Letters 7, 1643 (2007).
[2] J. H. Chen, C. Jang, M. S. Fuhrer, E. D. Williams, and M. Ishigami, Nature Physics, 4, 377 (2008).
[3] C. Jang, S. Adam, J.-H. Chen, E. D. Williams, S. Das Sarma, M. S. Fuhrer, Physical Review Letters 101, 146805 (2008).
[4] J. H. Chen, C. Jang, S. Xiao, M. Ishigami, M. S. Fuhrer, Nature Nanotechnology 3, 206 (2008).
[5] S. Cho and M. S. Fuhrer, submitted.

19:00

Graphene quantum dots

Christoph Stampfer[1] Johannes Güttinger[1] Tobias Frey[1] Stephan Schnez[1] Françoise Molitor[1] Sarah Hellmüller[1] Thomas Ihn[1] Klaus Ensslin[1]
[1]Nanophysics Group, ETH Zurich, Zurich

Graphene, the first real two-dimensional solid consisting of a hexagonal lattice of carbon atoms reveals a number of unique electronic properties making this material interesting for high mobility electronics, spintronics and nanoelectronics in general. Here we report on measurements showing that excited single-particle states can be detected in graphene quantum dots via co-tunneling in the Coulomb blockade as well as via related conductance resonances at high voltage bias outside the blockaded regions. The devices, consisting of graphene islands with diameters of around 50 to 140 nanometers are connected via two narrow graphene constrictions to source and drain contacts. These devices are tunable by lateral graphene gates. From transport measurements we extract charging energies around 10 meV and single-level spacings of a few meV. We demonstrate the functionality of a charge-read-out using a nearby graphene constriction. Both steps, the detection of excited states and the charge-read-out, are crucial for the investigation of graphene quantum devices in general as well as for future implementations of spin qubits in graphene.

19:30

Molecular states of correlated electrons in quantum dots

Massimo Rontani
CNR-INFM Research Center S3, Modena, Italy

The electron-electron interaction is predicted to fundamentally affect electron states in quantum dots (QDs), giving rise -in certain regimes- to a molecule made of electrons, whose mutual distances are rigidly fixed like those of nuclei in conventional molecules.

We first report evidence of molecular behavior based on inelastic light scattering measurements of the excitations of low-density GaAs quantum dots containing exactly four electrons. Theoretical predictions obtained via the configuration interaction (CI) method are in quantitative agreement with the observed excitations and highlight that roto-vibrational modes develop at the onset of short-range correlation.

We then investigate QDs in carbon nanotubes, which provide dramatic evidence of correlation. Our CI calculations take into account the role of two-valley degeneracies as well as the spin-orbit interaction. Without spin-orbit, the two-electron ground state is a triplet, due to the occurrence of a pseudospin degree of freedom linked to the orbital degeneracy. By including spin-orbit, we demonstrate that Coulomb correlation is an essential feature for explaining recent single-electron tunnelling spectra.

1

New NMR strategies to study carbon nanotubes

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[2]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA
[3]Department of Physics, Umeå University, S-901 87 Umeå, Sweden
[4]European Theoretical Spectroscopy Facility (ETSF), Dpto. Física de Materiales and Centro Mixto CSIC-UPV/EHU, Universidad del País Vasco UPV/EHU, Edificio Korta, Avd. Tolosa 72, 20018 San Sebastián, Spain

The local magnetic properties of the one dimensional inner space of the nanotubes are investigated using ^{13}C nuclear magnetic resonance spectroscopy of encapsulated fullerene molecules inside single walled carbon nanotubes. Isotope engineering and magnetically purified nanotubes have been advantageously used on our study to discriminate between the different diamagnetic and paramagnetic shifts of the resonances. Ring currents originating from the π electrons circulating in the nanotube, are found to actively screen the applied magnetic field by -36.9 ppm. Defects and holes in the nanotube walls cancel this screening locally. At high magnetic fields, the modifications of the NMR resonances of the molecules from free to encapsulated can be exploited to determine some structural characteristics of the surrounding nanotubes.

2

Helicities sorting of single-walled carbon nanotubes by amphiphiles molecules adsorption studied by resonant Raman excitation profiles

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Adsorption of specifically designed polyaromatic amphiphiles were used to sort single-walled carbon nanotubes (SWNTs) with different helicities. The sorting is investigated by resonant Raman excitation profiles. Chiral indexes (n and m) of SWNTs present in our samples are determined by fitting the Raman peaks observed in the radial breathing modes region (RBM). Scanning over an excitation energy range between 2 and 2.2 eV with a 0.01 eV step allows to investigate mainly two families of metallic nanotubes (2n+m=24 and 2n+m=27). The results display significant differences between the sorted and the reference samples, meaning that

discrimination between SWNTs of different helicities is possible.

3
Improving Quality of Single Walled Carbon Nanotube Networks

Alberto Ansaldo[1] Sandesh Jaybhaye[1,2] Marco Chiarolini[3] Ermanno Di Zitti[3] Davide Ricci[1]
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Single walled carbon nanotubes (SWCNTs) are one of the most interesting materials for transparent conductive films. SWCNT percolating networks have been produced by a variety of different methods mainly by spraying and filtration. Unfortunately, suspending CNTs in liquid requires the use of ultrasound and surfactants. Sonication reduces bundling but increases the number of defects and shortens CNT length. Moreover, after deposition, surfactants are difficult to be removed and tend to create an insulating layer between CNTs and between CNTs and contacts. The overall effect is to considerably reduce the global conductivity of CNT films. It is our opinion that a considerable improvement in film quality could come from a direct synthesis of the network by chemical vapour deposition (CVD) and combining this with direct transfer techniques that avoid suspension of the CNTs in a liquid. In this work we show our latest results in enhancing the quality of SWCNT percolating network synthesis by alcohol CVD on silicon oxide substrates using cobalt and nickel acetates as precursors, varying catalyst composition, substrate preparation and catalyst pre-treatment.

4
Engineering the spin transport in graphene with vacancies

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We use densiy functional theory to study in detail the magnetic structure of monovacancies in graphene. Breaking of sublattice symmetry leads to spin polarization, coming from both localized and delocalized states. We propose arranging the vacancies in one-dimensional 'tracks' as a pathway to create novel spintronic circuit elements with highly tunable properties, based entirely on graphene. We also study the effects of chemical modification of vacancies with different species (H, F, B, N) to saturate the reactive dangling bonds; controlled cemical modification is proposed as an additional tool to alter the magnetic structure of graphene.

5

Continuum Elastic Modeling of Graphene Resonators

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Starting from an atomistic approach, we have derived a hierarchy of successively more simplified continuum elasticity descriptions for modeling the mechanical properties of suspended graphene sheets. We find that already for deflections of the order of 0.5 Å a theory that correctly accounts for nonlinearities is necessary and that for many purposes a set of coupled Duffing-type equations may be used to accurately describe the dynamics of graphene membranes. The descriptions are validated by applying them to square graphene-based resonators with clamped edges and studying numerically their mechanical responses. Both static and dynamic responses are treated, and we find good agreement with recent experimental findings.

6

Photoemission and x-ray absorption studies on magnetic rare earth metallofullerenes and ErCl3 nanowires inside carbon nanotube templates

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Magnetic rare earth metallofullerenes and crystalline ErCl3 nanowires templated inside carbon nanotubes can be tailored under high temperature and vacuum with a high filling-ratio yielding novel magnetic chains and quantum wires [1,2]. A combination of resonant photoemission and XAS has been utilized to assess the charge transfer and bonding environment in the pristine nanotube templates and the filled functionalized separated samples [3]. Core level information of the filler is investigated to reveal hybridization state and bonding environment of the elements in these structures. Resonant PES is also studied in order to discern the metallicity of the filler. This allows us to evaluate the changes in the electronic structure of the valence and conduction band of the CNT. For the latter additionally, XPS line shape analysis will also be discussed for a detailed analysis of the chemical state and bonding environment.

Work supported by the DFG PI 440 3/4/5.

[1] R.Kitaura and H.Shinohara, Jap.J.Appl.Phys.46 (2007) 881

[2] R.Kitaura et al. NanoRes 1(2008)152

[3] T.Pichler et al. Phys.Stat.Sol.b 245(2008) 2038

7

Carbon Nanotube Synthesis via Ceramics

A. Bachmatiuk[1] M. Bystrzejewski[2] P. Ayala[3] F. Schaeffel[1] E. Borowiak-Palen[4] A. Huczko[2] H. Lange[2] T. Gemming[1] T. Pichler[5] C. Mickel[1] R. Klingeler[1] H-W. Hübers[6] M. H. Rümmeli[1]
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[3]Laboratory of Physics and Center for New Materials, Helsinki University of Technology, Finland
[4]Szczecin University of Technology, KnowMatTech, Szczecin, Poland
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[6]German Aerospace Agency (DLR), Adlershof, Berlin, Germany

The potential for ceramics as catalysts for CNT formation exceeds that from metal catalysts in that ceramics can serve as a catalyst particle for CNT nucleation/growth as found with metal catalysts. In addition, they can also serve as a template for the synthesis of carbon nanostructures. This latter point (template route) provides a more versatile means to engineer different types of nanotubes structures (e.g. Y junctions), as compared to metals catalysts. Furthermore, ceramics are often removed (purification) from as produced samples far more easily than metal catalysts. Here we present studies on the growth of carbon nanotubes (CNT) from ceramics in chemical vapour deposition (CVD) and laser pyrolysis routes. We show CNT growth from both ceramic particles and nanowires. The nanowires serve as templates. Further, we demonstrate the templating route can also be used for doping (B) the CNT.

8

Solubilization and Density Gradient Fractioning of SWCNTs by a Novel three Component Surfactant Class Based on Perylene Dyes

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[1]Institute of Advanced Materials and Processes, University Erlangen Nurenberg
[2]Department of Chemistry and Pharmacy, University Erlangen Nurenberg

For exfoliating SWNTs, we have developed a three component surfactant with solvophylic moiety, polycyclic aromatic perylene bisimide unit for interaction with the SWNT backbone and hydrophobic aliphatic tail. The degree of individualization of the SWNTs is higher than for dispersions in the commonly used surfactant SDBS as shown by statistical AFM analysis. Furthermore, optical spectroscopy revealed dispersion and individualization at a SWNT to perylene (Per) weight ratio of 2:1. The SWNT-Per dispersions were characterized by various spectroscopic and microscopic techniques. A π -stacking interaction is reflected by a redshift of the optical perylene transitions, a strong alteration of the SWNT emission pattern and a significant quenching of the SWNT and perylene fluorescence intensity (C. Backes, et. al., J. Am. Chem. Soc., accepted).

We have applied this surfactant in density gradient ultracentrifugation (DGU) separation experiments where a high degree of SWNT individualization is a key to success. SWNTs were fractioned in a combined co-surfactant and replacement DGU approach underlining the versatility of our dispersion concept (C. Backes, et. al., Chem. Commun., accepted).

9

Carbon Nanotube CVD on a Tantalum support for Interconnect Fabrication â materials interactions

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[1]Engineering Department, University of Cambridge, Cambridge, UK
[2]Sincrotrone Trieste S.c.p.A., Area Science Park, Trieste, Italy
[3]Laboratorio Nazionale TASC-CNR-INFM, Trieste, Italy

A possible application for carbon nanotubes (CNTs) is the use as interconnects in large scale integrated (LSI) circuits [1]. However, the deposition process must yield vertically aligned, high density CNTs on conductive materials and must be compatible with commonly used LSI materials.

In this study we examine the growth of CNTs by thermal chemical vapour deposition (CVD) on LSI-compatible Ta support layers with an iron catalyst. Structural and morphological characterisation of the obtained CNT forests and the support/catalyst system is undertaken to gain insight into possibly growth-inhibiting reactions of the Ta support layer, the metal catalyst layer, the process gases and residual gases in the CVD system and their temperature dependence. In addition, X-ray photoelectron spectroscopy (XPS) is used to resolve chemical interactions directly at the interface of the buffer layer, the catalyst and the growing CNTs. This is compared to CNT growth on commonly used oxide supports [2].

[1] Robertson J. et al., Appl Phys Lett, 93, 163111-1, 2008
[2] Mattevi C. et al., J Phys Chem C, 112, 32, 12207, 2008

10

Multi Walled Carbon Nanotubes Plastic Actuator

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Carbon nanotubes have electrical and mechanical properties that make them highly attractive for actuators. They have the ability to deform elastically by several percent, thus storing very large amounts of energy, thanks to their crystalline nature and to their morphology. A bimorph actuator composed of single walled carbon nanotubes (SWCNTs), polyvinylidene difluoride (PVDF) and the ionic liquid (IL) 1-butyl 3-methylimidazolium tetrafluoroborate [BMIM][BF_4] with a polymer-supported internal ionic liquid electrolyte was previously demonstrated by Aida et al.[1]. While several experiments were carried on using SWCNTs, PVDF and a number of ILs, the use of multi walled carbon nanotubes instead of SWCNTs is, to our knowledge, a new result that will be presented here. Electrochemical characterizations by cyclic voltammetry, impedance spectroscopy and actuation tests performed applying a square wave of 4 Volt peak-to-peak at frequencies between 0.3 Hz and 2 Hz will be reported and discussed.

[1] T.Fukushima, T.Aida, âIonic Liquids for Soft Functional Materials with Carbon Nanotubes,â *C*hem.Eur.J., vol. 13, no.18, pp. 5048-5058, Jun. 2007

11

Strongly Correlated Electron Phenomena in Carbon Nanotubes

Marc Bockrath[1] Vikram V. Deshpande[1] Bhupesh Chandra[2] Robert Caldwell[2] Dmitry Novikov[3] James Hone[2]
[1]California Institute of Technology, Pasadena
[2]Columbia University, New York
[3]Yale University, New Haven

In this talk I will discuss our recent results demonstrating strongly correlated electron behavior in ultra-clean carbon nanotube quantum dots. Specifically, we have observed one-dimensional (1D) Wigner crystal behavior of dilute holes in semiconducting nanotubes, finding three distinct regimes of spin and valley quantum number ordering as the charge density and axial magnetic field are varied. The boundaries between the regimes in density and magnetic field are well-described by the theory of Levitov and Tsvelik for a narrow-gap Luttinger liquid. In the second part of the talk I will present results showing that the electrons in nominally metallic nanotubes comprise a 1D Mott insulator. This indicates that carbon nanotubes are never truly metallic, in agreement with theoretical predictions that account for umklapp scattering at half-filling due to electron-electron interactions. Using inelastic cotunneling spectroscopy, we also observe neutral electronic excitations within the gap, yielding an additional signature of strong electron-electron interactions. Our results demonstrate nanotubes' promise for studying a variety of tunable correlated electron phenomena in 1D.

12

Tailoring carbon nanotubes grown from non-ferromagnetic catalysts via CVD.

Ewa Borowiak-Palen[1] A. Steplewska[1] A. Bachmatiuk[1] M. H. Rümmeli[2] R. J. Kalenczuk[1]
[1]Institute of Chemical and Environment Engineering, Szczecin University of Technology, Szczecin
[2]2. Leibniz Institute of Solid State and Materials Research Dresden, Germany

The catalytic growth of different carbon nanotubes by chemical vapor deposition (CVD) using non-ferromagnetic catalyst particles (such as copper) will be presented. In this work detailed studies that catalysts with fully filled d orbital (e.g. Cu) can be a source of bulk scale synthesis of singlewalled or multiwalled carbon nanotubes using the same catalyst mix (viz. equal molar ratio of metal to magnesia) but with different experimental setups and conditions. The detailed analysis of the samples is supported by electron transmission microscopy observations, energy dispersive X-Ray spectroscopy mode, X-Ray Diffraction and Raman spectroscopy.

13

Various methods of surface-enhanced Raman spectroscopy applied to single and double walled carbon nanotubes

Bea Botka[1] Katalin Kamaras[1]
[1]Research Intitute for Solid State Physics and Optics, Budapest

We investigated several SERS (surface-enhanced Raman spectroscopy) methods reported in the literature regarding their application to carbon nanotubes. Silver and gold were used to prepare different types of surfaces. We achieved surface enhancement factors up to 200 by a modification of the method by Ouyang and Fang [1] on silver. In particular, we were able to detect with enhanced sensitivity the intermediate frequency modes (Z-breathing phonons), which correspond to vibrations along the nanotube axis, and which, according to theoretical predictions [2], are sensitive to the nanotube length. These modes are usually weak or non-existent in the normal Raman spectra. We will compare these modes in several types of nanotube samples, and demonstrate the effect of physical and chemical treatment.

Supported by the European Commission FP7 through the Initial Training Network FINELUMEN, contract PITN-GA-2008-215399.

[1] Y. Ouyang, Y. Fang: Spectrochimica Acta Part A 61 (2005) 2211â2213
[2] R. Saito et al. : Phys. Rev. B 59 (1999) 2388-2392

14

Polarized Raman measurements on the reaction center of crystallized photosystem II

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[1]Festkörperphysik, Technische Universität Berlin, Berlin
[2]Institut für Chemie, Technische Universität Berlin, Berlin

In photosynthesis the sunlight is collected by antenna pigments and transmitted to special molecule structures called photosystem I and photosystem II, where the energy of light is transformed into a separation of charge. In the photosystem II reaction center, two β-carotene molecules Car$_{D1}$ and Car$_{D2}$ were identified, which are oriented perpendicular to each other^1. The role of these carotenes in the photosynthesis process is still unknown. We use Raman spectroscopy, which is one of the most important methods to analyse the structure of solids and molecules, to study the two β-carotenes. We present polarized Raman measurements of the *beta*-carotene vibrational modes in single crystals of photosystem II and discuss the possible origin of the observed polarization dependence.

15

A Molecular ^{15}N Quantum Nuclear Memory using ^{15}N@C$_{60}$

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N@C$_{60}$ is of significant interest in the quantum information processing (QIP) community due to its long electron decoherence times and ability to be incorporated into larger computing architectures. In QIP the loss of information through the process of decoherence is a fundamental problem, but it can be combated through the transfer of qubit (quantum bit) states. Electron spins allow fast manipulation and are easily initialised compared to nuclear spins, but suffer from short decoherence times. Nuclear spins have significantly larger decoherence times than electron spins and hence propagation of states can provide a route to information storage. Thus, a powerful model would use the electron qubit for initialisation, processing and readout, with transfer to a nuclear 'memory' qubit. We have implemented such a scheme using a series of tuned microwave and radiofrequency pulses to produce a ^{15}N nuclear memory within a dilute ^{15}N@C$_{60}$ in C$_{60}$ matrix. The work reports a significant improvement in decoherence time of over two orders of magnitude through information transfer from the electron to the nuclear spin state, with a two-way fidelity of 70%.

16

COMPARATIVE STUDY OF THE ELECTRONIC STRUCTURE OF DIFFERENT TYPES OF SINGLE-WALL CARBON NANOTUBES

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[2]AIST, Tsukuba, Japan
[3]Max-Planck-Institute for Solid State Research, Stuttgart, Germany
[4]Laboratoire de Chimie et dâElectrochimie des Surfaces, FUNDP, Namur, Belgium

Electronic structure of single-wall carbon nanotubes (SWNTs) has been probed by near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Three types of SWNT samples were examined: SWNTs produced by laser vaporization method, SWNTs synthesized by methane decomposition over Co catalyst supported on MgO, and aligned SWNTs produced on silicon support using a super-growth method. Alignment of the third type of SWNTs was determined from an angular dependence of a ratio of π^* and σ^* resonances. The width of angular distribution of SWNTs in a film exceeds the value found from SEM image analysis that could be due to defects in SWNTs. Defects should contribute to the NEXAFS spectrum and we found that π^* resonance width has the smaller value for laser-produced SWNTs and the larger value for aligned SWNTs. X-ray absorption spectra of armchair, zigzag and semiconducting chiral carbon nanotubes were modeled based on the results of B3LYP calculations. It was shown that the geometry of carbon nanotubes has effect on the width of the π^* resonance. Thus, NEXAFS spectroscopy could be used for checking of a presence of metallic SWNTs in a sample.

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Characterisation of cobalt(II)porphyrin/carbon nanotube nanohybrids by electron paramagnetic resonance and optical spectroscopy

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In this study, we use electron paramagnetic resonance (EPR) spectroscopy in combination with absorption, steady state and time resolved fluorescence spectroscopy to characterize paramagnetic cobalt(II)octaethylporphyrin (CoOEP)/single-wall carbon nanotube (SWNT) nanohybrids.[1] While measuring on a bulk sample, two different components can be distinguished in the EPR spectrum, arising from porphyrins interacting with metallic and semiconducting NTs. From analysing these two EPR contributions, we conclude that the metallic NTs are stronger π-acceptors for the porphyrins than the semiconducting NTs. Solubilising the nanohybrids in water using bile salt surfactants[2], after applying a thorough washing procedure, yields stable solutions in which at least 99% of the porphyrins are adsorbed on the NTs. Thanks to this purification, we observe the isolated absorption spectrum of the interacting porphyrins, which is strongly red-shifted compared to the free porphyrin absorption, and a quasi-complete quenching of the porphyrin fluorescence.
[1] S. Cambré *et al.*, ChemPhysChem 2008, 9, 1930 [2] W. Wenseleers *et al.*, Adv. Funct. Mater. 2004, 14, 1107

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Manipulation of spin-active peapods for magnetic resonance studies

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Fullerene-like materials open up new fields in spin electronics because of their intrinsic characteristics as well as their ability to host species. Peapods, produced from spin-bearing endohedral fullerenes, enable to study spin-spin interactions, and spin transfer along spin chain. Herein, we will report on the fabrication of peapod-based devices for spin-chain analysis by Electron Spin Resonance (ESR) and electrically detected magnetic resonance (EDMR) for investigation of spin-dependent transport properties. Peapods are synthesized by sublimation of metallofullerenes in presence of single-walled carbon nanotubes which are produced by laser-evaporation process with non-magnetic catalyst, and sorted by electronic structure. Then, peapods are deposited onto substrates from organic solvent based-suspensions of debundled materials. Individual species as well as thin films with controlled orientation of the peapods can be obtained by means of dielectrophoresis. Finally, the integration of La@C82 peapods by use of electron-beam lithography into probe devices designed for magnetic studies will be presented.

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Improvement of Polypyrrole and Carbon Nanotube Co-deposition Techniques for High Charge-transfer Electrodes

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Both carbon nanotubes (CNTs) and polypyrrole (PPy) have been investigated as materials for manufacturing high charge-transfer electrodes due to their outstanding performances. The combination of the complementary properties of CNTs and PPy via an electrochemical co-deposition route has been already shown to achieve interesting results. In this work, PPy and chemically-functionalized multi walled CNTs (COOH-MWCNT) were potentiostatically, galvanostatically and potentiodynamically electrodeposited from an aqueous solution at different temperatures to form a nanocomposite on the surface of a variety of metal electrodes. A study of the influence of experimental parameters such as temperature, current, and growth rate in the different electrodeposition methods was performed. The electronic and electrochemical properties of the nanocomposite films have been studied by cyclic voltammetry and electrochemical impedance spectroscopy, while a morphological study has been performed via scanning electron microscopy. A comparison between

the different techniques will be reported and guidelines for best results depending on the application will be discussed.

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Atomic Diffusion and Reshaping of Solid Catalytic Particles During Nanotube Growth

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The catalytic particle dynamics during catalytic chemical vapor deposition of nanotubes (CNTs) plays a fundamental role in the nucleation and growth process and in the final CNT morphology. In-situ transmission electron microscopy videos at low temperatures show constantly reshaping solid catalytic particles [1,2]. Here, we explain the physics of this process and link it to the final CNT morphology. Using a combination of multiscale atomistic modeling and analytic continuum calculations we show that the reshaping can be either via surface diffusion or via bulk drift of the Ni atoms [3]. The temperature and the activity of the growing CNT edge determine the degree of surface diffusion or bulk drift. The nanoparticle reshaping is driven by capillary forces. The interplay between the capillary and anchoring forces can lead to either: 1)steady CNT growth, 2)encapsulation of the nanoparticle, 3)splitting of the nanoparticle, or 4)formation of bamboo-like CNTs. The physics in our study is elemental and general, and can be extrapolated to other nanosystems.

1 S. Hofmann, et al. Nano Lett, 7 602 (2007)
2 S. Helveg, et al. Nature, 427 426 (2004)
3 F. Cervantes-Sodi et al submitted (2009)

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METALLIC SINGLE-WALL CARBON NANOTUBES SEPARATED BY DENSITY GRADIENT ULTRACENTRIFUGATION

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Unique properties of single wall carbon nanotubes (SWNTs) are already successfully used in technologies. Depending on geometry SWNTs may be either metallic or semiconducting. Up to now synthesis is not able to provide a purely metallic nanotube fraction. A recent method of a density gradient ultracentrifugation (DGU) is efficient in separation of SWNTs. In this work we used DGU to extract a metallic fraction from as-grown arc-discharge SWNTs. The process parameters (the surfactant type and concentration, the treatment time, the approach to the gradient formation) have been optimized. The metallic fraction has appeared as an upper one, colored in blue. The fraction has been studied with the UV-VIS-NIR

absorption and Raman techniques. The only one absorption band (with maximum at 680 nm) corresponding to metallic nanotubes has been observed. The results obtained are important for formation of the optical media with desired properties [1], especially for nanoelectronics and laser physics [2].

Thanks for support with RFBR-07-02-91033 and RAS programs.

1.A.I. Chernov et al., Phys. Stat. Sol. (b), 244 (2007) 4231.

2.A.V. Tausenev et al., Appl. Phys. Lett. 92 (2008) 171113.

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Electron spin resonance study of graphene flakes

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Electron spin resonance (ESR) is an efficient technique to study the density of states (as a function of temperature and doping) of graphene, and to detect magnetic interaction of localized spins at the edges of graphene flakes and ribbons. We have performed ESR measurements in the 4-300 K temperature range on graphene samples derived from: 1) chemical reduction of graphene oxide sheets, 2) liquid phase exfoliation of graphite (LPEG), 3) and mechanical exfoliation. The ESR signal depends very much on the method of preparation of graphene. The amount of localized spins and the Pauli component of the spin susceptibility vary from sample to sample. In some cases stronger-than-Curie temperature dependence is observed below 20 K. We will report preliminary ESR experiments on K- and N-doped graphene samples, as well.

Acknowledgment: The work is performed in collaboration with R. Nesper, J. Coleman and K. Kern. The project is partially supported with the European Network IMPRESS.

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Single Molecule Circuits with Carbon Nanotube Wiring

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The vision for molecular electronics extends well beyond miniaturation and scaling to include new techniques for studying chemical bonding, biocatalysis, and molecular recognition. However, operational single molecule devices remain exceedingly fragile and difficult to fabricate. We have demonstrated a promising new architecture for studying single molecule behavior based on point functionalizationöf single-walled carbon nanotube circuits. In this technique, single defects are created in the sidewall of an electrically connected nanotube. The technique, free of precision lithography or mechanical manipulation, produces single attachment sites in operational circuits, and enables the electrical monitoring of single molecule dynamics. This presentation will describe these techniques and demonstrate real-time, single molecule monitoring of various chemical processes including oxidation, conjugation, recognition and binding. Advantageous properties of the nanotube architecture include excellent electrical, mechanical, and chemical stabilities and well-defined bonding to the molecules of interest.

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Raman spectroscopy study on concentrated acid treated carbon nanotubes

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Aggressive purification treatments may modify the carbon nanotubes (CNTâs) electronic and vibrational properties. The most common procedures to remove catalyst particles in the raw carbon materials involve the use of acids, either individually or in different combinations, through long periods of refluxing and/or sonication processes. A comparative study will be presented on the effect of strong acid treatments either in single walled (SWCNT's) and multi walled carbon nanotubes (MWCNT's). The effects were studied by Raman spectroscopy, well known as a powerful tool in the characterization of the electronic and vibrational modes of CNTâs. The results show that in SWCNTâs the raw sample shows a broader G band, well fitted using a Breit-Wigner-Fano (BWF) line in comparison with the acid treated sample, which can be fitted using a Lorentzian lineshape. The original shape of this feature is recovered after the annealing step. With respect to the MWCNTâs samples, an increase in the intensity of a second peak in the Gâ band region was observed after the acid treatment. The origin of this double peak is not yet clarified.

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Gate-tunable ferromagnetic proximity effect and giant g-factor fluctuation in InAs Nanowire Quantum Dots

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Semiconductor nanowires (NW) provide new alternatives to fabricate quantum electronic devices. The possibility to contact InAs NWs with ferromagnetic (F), superconducting (S) and normal (N) electrodes, to implement local gates, and the strong internal spin-orbit interaction allow exploring novel transport effects of hybrid nanostructures. We study InAs NW quantum dots using both N, F, S contacts, and explore the spin physics by measuring the B field-induced splitting of the spin 1/2 Kondo effect. Unlike to previous studies, the g-factors of neighboring states

can scatter between 2 and 18 and can therefore be even larger than in the bulk (g=15). We demonstrate further the electric gate tunability of the g-factor in a single charge state. When using F contacts a zero-field splitting is induced. This proximity induced exchange field has recently been measured for the first time by Hauptmann et al. (Nature Physics Vol 4, (2008)) in carbon nanotubes. Here, we show the same effect in a semiconducting NW, demonstrating that this effect is universal. Employing a pair of S and F contacts, the proximity-induced exchange shows up as a âkleineâ-gap in superconducting spectroscopy.

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Study of the role of Fe based catalysts on the growth of B-doped SWCNTs synthesized by CVD

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The production of B-doped single-walled carbon nanotubes by chemical deposition methods has only recently been successful. The complex interplay within the thermodynamic parameters added to the favorable formation of solid compounds containing Boron, have generally made of this synthesis a difficult task to achieve. This contribution will mainly focus on the role of the catalyst composition as one of the crucial parameters to produce the B-doped single wall carbon nanotubes by chemical vapor deposition. In this study, we point out the effect of Fe based catalysts, which were prepared from different kinds of Fe compounds supported in different porous magnesium oxide powders comparable to the traditional synthesis of pristine carbon nanotubes. Not only the quality and the yield of nanotubes produced with each catalyst were studied, but also the formation of by products was carefully monitored. Transmission electron microscopy and Raman spectroscopy have been used to analyze the overall nanotube quality, whereas XRD and analytical electron microscopy have been used in order to determine the catalysts composition before synthesis and the formation of byproducts after the reactions occur.

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Photoselective resonant Raman response of n- and p- type intercalated graphite and SWCNT revisited

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We present new studies on the detailed photoselective Raman response of n- and p-type intercalated graphite and SWCNT. Here we focus on the high doping region. The shift of the G line is used to monitor the doping level of the potassium doped graphite intercalated compounds (GIC) and the p- type intercalated SWCNT using irontrichloride. Special emphasis is given on the charges in the dispersion of the D and D* lines as a function of doping.We also discuss the implications of our results on the doping induced modifications in the Kohn anomaly in the phonon dispersion at the K point. Acknowledgements: DFG PI 440-5.

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Preparation and characterization of LiMnPO4/SWNT composites as cathode material for Li-ion battery.

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The olivine type materials, like LiMnPO^4 , are considered as cathode materials for the lithium ion batteries. Due to their low electrical conductivity usually up to 40 wt % of conductive additive in form of carbon black is required. The additive does not participate in the electrode reactions and therefore represent a dead weight reducing the storage capacity. We replaced the state-of-the-art carbon coating by in situ incorporation of functionalized carbon nanotubes. Compared with blank LiMnPO4 nanoparticles, much finer nanoparticles with higher surface area were produced in the presence of nanotubes. This observation indicates that functional nanotubes play an important role for nanoparticle nucleation, and coagulation processes. Whereas the electrical conductivity of the composite increases by 5 orders of magnitude upon addition of only 1 wt % of SWNT, the battery capacity with a value of 20 mAh/g appears low. The SWNT with their high aspect ratio are forming a percolating network through the composite at a low concentration, but do not suppress the agglomeration of LiMnPO4 nanoparticles, which limits the Li-ion mobility and leads to only modest electrochemical performance.

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New carbon nanostuctures formed on the surface of carbon fiber by laser radiation

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We have developed a method of growing nanocarbon particles on the surface of carbon materials. To do this, the surface of carbon fibers were radiated by a laser in a carbon content gas atmosphere. A new carbon nanoparticle containing a combination of nanostructures was discovered. These new nanomaterials possess unique mechanical, electrical and thermal characteristics and can be used in a wide range of applications in different areas from new high strength materials, to photo electronics and lighting. These nanostructures have been studied using electron diffraction and high-resolution electron microscopy, and their mechanical characteristics were tested, as well.

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Silicon Carbide Nanowires: Synthesis and Cathodoluminescence

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The betaâSiC nanowires were efficiently produced using the thermal-explosion mode of selfâpropagating high temperature combustion synthesis (SSH) from elemental Si and poly(tetrafluoroethylene) powder mixtures combusted under different operational parameters [1]. The report presents the study of one- dimensional silicon carbide structures by means of cathodoluminescence (CL) technique [2]. CL spectra of several nano 1D-SiC samples and of a reference commercially available 3C-SiC, measured at 77 K, are compared. It was demonstrated that the emission band at 1.97 eV related to irradiative transitions between the deep defect level (silicon vacancy) and the conduction band (weakly detected in the spectrum of the commercial SiC) becomes, under 10 keV electron beam irradiation, the prevailing band in CL of the purified silicon carbide nanowires. After the final stage of purification process the intensity of 1.97 eV band is almost 10 times stronger with respect to the 2.38 eV peak which, in turn, corresponds to band-to-band transition in 3C-polytype of silicon carbide. Observed behavior confirms that produced nanowires are defects-enriched. 1. A. Huczko et al., J. Phys.: Condens. Matter 19, 2007, 395022. 2. S. Bellucci et al., Radiation Measurements 42, 2007, 708.

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SFM manipulation techniques applied to graphene

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Graphene is a promising candidate for future generation electronic devices. Methods which allow its structuring and its manipulation are needed for the development of possible applications. Thinness, flexibility and flatness of graphene render SFM techniques promising for single or multilayer graphene. Here we demonstrate two approaches using a scanning force microscope (SFM) tip. First, manipulation of graphene is investigated, particularly „sawing“which produces nangaps and nanoribbons as well as manipulating parts of graphene without destruction. In all these cases the manipulation is carried out on graphene in contact with SiO2 substrates. Near a graphene edge or when the graphene is small enough it can be desorbed and turned with the SFM-tip since the adsorption force between graphene and the substrate is smaller than the force to break the graphene. Second, adsorption and manipulation of DNA on an amphiphile interlayer is presented. The interlayer is needed to provide the proper DNA mobility such that it can be manipulated. It is shown that a force can be found large enough to manipulate DNA but too small to damage the graphene.

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Actuation of arrays of vertically aligned carbon nanotubes

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Arrays of vertically aligned carbon nanotubes were grown on Mo electrodes. By applying a DC-bias we successfully actuated these arrays. This effect can be used to make varactors.

Videos of the actuation were recorded in an optical microscope. In order to study the actuation in more detail and with larger depth of focus the nanotube arrays were also actuated in a SEM.

The voltage was increased to just below the pull-in voltage, where the arrays come in contact with each other and the device is destroyed. The voltage was then lowered in order to separate the arrays and then increased again. This procedure could be repeated up to 15 times without any significant degradation.

The capacitance between the arrays was measured by measuring the s-parameters of the devices. The initial capacitance of a device was measured to 22 fF. During actuation the capacitance could reproducibly be increased by over 20%.

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Thin Film Nanotube Transistors Based on Self-Assembled, Aligned, Semiconducting Carbon Nanotube Arrays

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Thin film transistors (TFTs) are poised to revolutionize the display, sensor and flexible electronics market. Channel materials so far have been mainly organics and amorphous silicon, which have limited carrier mobilities. Single-walled carbon nanotubes have extremely high mobilities and can be solution processed, which makes thin film CNT based TFTs a natural direction for exploration. Here we address two main challenges facing CNT-TFTs: low on/off ratios because of admixture of metallic nanotubes, and the placement and alignment of CNTs over large areas. We reduce the content of metallic nanotubes to 1% by density gradient ultracentrifugation [1] confirmed by optical and electrical measurements. The deposition problem is addressed by self-assembly of nanotubes in stripes to produce dense and aligned CNT films over large areas at room temperature. Transistors fabricated on such films show good drive currents and high on/off ratios. Additionally, these devices exhibit strong photocurrents and are both photo- and electroluminescent, which hints at possible optoelectronic applications [2]. [1] Arnold et al., Nature Nano, 2006, 1(1), 60 [2] Engel et al., ACS Nano, 2008, 2(12), 2445

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Individualization of Graphenoid Building Blocks in Aqueous Solutions

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Due to the highly versatile bottom up approach towards well defined monodisperse graphenoid building blocks, investigations concerning the aggregation of such building blocks like hexa-peri-benzocoronenes (HBCs) may shed light into the development of methods to overcome the mutual attractive π -stacking interactions in such polyaromatic hydrocarbons.

Inspired by the research on CNT solubilisation by the use of surfactants, herein we report on the individualization of unsubstituted, highly insoluble HBC discs in water by different detergents: Sodiumdodecylbenzenesulfonate, Sodiumcholate, Sodiumdeoxycholate and amphiphilic perylenebisimides derivatives were used in combination with mild ultrasonication.

Analysis of HBC so far was only possible by means of derivatisation to overcome the intrinsic insolubility in all common solvents. Our approach abstains from direct chemical modification. To examine the aggregation state of the dispersed material UV/Vis absorption and photoluminescense spectroscopy were utilized. Upon applying sedimentation theory we found different decay constants for the surfactants used indicating varying efficiency for the systems under investigation.

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Growth of carbon nanotubes on mono- and poly-crystalline Si substrates

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In microelectronics, carbon nanotubes (CNTs) are envisaged as interconnects in vias and between transistors. For this application, densely-packed bundles of CNTs with predefined properties and orientations must be contacted, and preferably (surface-bound) grown, onto conductive materials. Herein we report the direct growth of CNTs by catalytic chemical vapour deposition onto two conductive Si-based substrates. By systematically evaluating pre-treatment conditions on 0.5, 1, and 1.5 nm of Ni, Co, and Fe, we demonstrate the growth of CNTs with interconnects requirements onto highly doped mono- and poly-crystalline Si substrates. This growth is effectively achieved only when the catalyst materials are restructured by plasma-assisted thermal pre-treatment. In the absence of this plasma assistance, i.e., just by purely-thermal pre-treatment, only uncontrollable growth is observed. The key role of the plasma is to produce active nanoparticles at lower temperatures than those typically used in purely thermal conditions. These nanoparticles induce isotropic CNT growth in the tube length direction with high degree of homogeneity in morphology and vertical-alignment perpendicula

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Large Scale Production of Graphene Nanoribbons by Nanowire Lithography

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Graphene nanoribbons (GNRs) are the counterpart of nanotubes in graphene nanoelectronics. The search for a cheap, parallel and deterministic technique for practical implementation of these structures is still open. Nanowire-lithography (NWL) consists in using NWs as etch masks to transfer their one-dimensional morphology to an underlying substrate [1,2]. Here, we show that oxidised silicon NWs (SiNWs) [3] are a simple and compatible system to implement the NWL concept on graphene. The SiNWs morphology is transferred onto a graphene flake by a low-power O2 plasma in a deep-reactive-ion-etcher [4]. The process leads to conformal GNRs with diameter comparable to the overlaying NW lateral dimensions. The diameter can be further reduced by multiple O2 etching steps. Raman spectroscopy is used to characterise the structure of the resulting GNRs. Field-effect measurements show the transition to a semiconductor when low diameters are reached. The influence of trap states on the device performance is discussed.

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2. D.Whang, et al. Nano Lett. 3, 951 (2003)
3. A.Colli, et al. J. Appl. Phys. 102, 034302 (2007)
4. A.Fasoli et al. submitted (2009)

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Ab-initio investigation of thermo activated directional transport of hydrogen molecules inside narrow carbon nanotubes

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The potential profiles for H2 molecule movement inside narrow single-wall carbon nanotubes ((3,3), (6,0) and (7,0)) have been calculated by DFT calculations. This potential forms a goffered potential surface with magnitude 160,1025 and 365K correspondently. We show that in these SWCNT transport of H2 molecules is given mainly by thermo activated hopping between minima of the periodic potential along the tube axis. At that the hopping rate of H2 molecules may be calculated by the Vineyard formula: $\omega = \frac{\prod_{\lambda}{}^{\omega_\lambda}}{\prod_{\lambda}{}^{\omega\hat{a}_\lambda}} \exp(-\frac{V_0}{kT})$ in which frequencies of vibrations correspond to positions of H2 at minimum and saddle point of the CNT potential. Modeling the temperature change ($\sim$ 300K) along the SWCNT with length ($\sim 1\mu$km) and using model of hopping at not uniform hydrogen density inside these CNT we show that H2 molecules would move in direction of the temperature decreasing. At that we show that H2 density close the both CNT ends would differ at $\sim$ 10 times. We hope that this effect is possible to use for build up a molecular pump driven by the temperature gradient along nanotube.

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X-RAY DIFFRACTION STUDY OF WS2 NANOPARTICLES AND NANOTUBES INTERCALATED BY ALKALI METALS (Na, K, Rb)

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WS2 inorganic fullerene-like (IF) nanoparticles were subjected to intercalation with potassium, sodium, and rubidium atoms in heated sealed ampoules. The product of the intercalation process was not pure and was composed of both intercalated and nonintercalated phases. Quantitative X-ray diffraction (XRD) analysis showed that after similar intercalation treatment the IF powder contained more of the intercalated phase than the 2H-WS2 material. XRD measurements under inert conditions of the intercalated powders showed that the interlayer expansion was correlated with the alkali metal radius. Small increase of the a-axis was observed as well and was explained on the grounds of the WS2 band structure.

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Sorting and transmission electron microscopy analysis of single or double wall carbon nanotubes

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Since there are many different structures of carbon nanotubes inducing different properties, several teams worked out different techniques to sort carbon nanotubes with respect to their structural properties such as diameter. However, until recently, the sorting efficiency has only been evaluated by probing optical or vibrational properties of sorted nanotubes. Since the relationship between these properties and the associated structure is not direct and not fully understood up to now, we propose here the structural analysis by TEM as a convenient and reliable way for evaluating the structural sorting of single or double wall carbon nanotubes. Furthermore, this approach allows us to determine the standard deviation of the carbon nanotube diameter distribution after sorting giving even more indications on the sorting process as well as on the carbon nanotubes optical properties (1). Possibilities and advantages of this approach will be demonstrated in the case of single walled and double walled nanotubes sorted by the gradient density technique.

(1) Fleurier et al, Adv.Func.Mater. 2008, submitted

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Hopping in carbon based nanostructures

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The temperature dependence of an assembly of carbon based nanostructures like: single and multi-walled carbon nanotubes, carbon onions, carbon nanoparticles, nano-horns, nano-graphite or flakes of graphene show a charge transport by hopping. Some of these systems have a similar behavior to graphene nanoribbons, where 1D variable range hopping conductivity was evoked. A detailed analysis and modeling of the conduction mechanism in all these systems will be presented.
The work is performed in collaboration with J. Coleman, R. Nesper, K. Kern and J.-P. Salvetat. It is partially supported by the European Network IMPRESS.

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Donor-acceptor nanocomposite structures for organic photovoltaic applications

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The performance of organic solar cells is mainly limited by the low transport properties of the applied organic materials. Particularly in bulk heterojunction device architectures it is the charge carrier transport which needs to be improved. We applied vacuum deposition techniques to prepare devices consisting of Zn-Phthalocyanine as donor and C60 as acceptor material. Co-evaporated donor-acceptor nanocomposites (DAN) were studied particularly with regard to their feasibility in organic solar cells. By modification of the deposition conditions like substrate temperature and deposition rate we could manipulate the DAN morphology and domain size, thus optimizing the device. The crystallinity of the individual domains was studied by means of transmission electron microscopy. The influence of the domain size on the cell parameters is discussed.

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Characterization of CNT thin-film transistors made of pristine and semiconductor-enriched SWCNTs

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Semiconducting single-wall carbon nanotubes (SWCNTs) are a candidate material for high-performance thin-film transistors (TFTs), because of their superior transport properties. Recently, we achieved enrichment of semiconducting SWCNT by a new separation method using agarose gel. In this work, we have fabricated a number of SWCNT TFTs using separated semiconducting SWCNTs (S-TFT) and compared the performance with that of pristine SWCNTs (P-TFT) without electrical breakdown treatment. SWCNT TFTs were fabricated by dropping a SWCNT dispersion in N-methylpyrrolidone onto a SiO2/Si substrate covered with self-assembled monolayer of 3-aminopropyltriethoxysilane, followed by depositing Au/Cr electrodes on it. The channel length and width were 10 and 200 um, respectively. SWCNT network structures in the channels of S- and P-TFTs were confirmed to be the same by AFM observation. For both S- and P-TFTs, about 20 devices were characterized. S-TFTs achieved 100 to 1000 times higher on/off ratios than those of P-TFTs without decreasing on-state current. This result indicates that the performance of TFTs was highly improved by using high purity semiconducting

SWCNTs.

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Optical Signature of Bundle Size Distribution in MoSIx Nanowire Dispersions

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Progress in nanotechnology crucially depends on molecular-scale materials with tunable physical or functional properties, yet with well-defined and controllable geometrical structure. MoSIx nanowires self-assemble into functional networks and qualify for applications as diverse as lubricant additives, field emitters, battery electrodes, (bio)chemical sensors, and as conductive or reinforcing component of composites. They disperse in many common solvents including water, where they occur in bundles of diameters ranging from a few 100 nm down to single wires (below 1 nm).

In this study we fractionated MoSIx nanowires by bundle diameter in liquid dispersion via centrifugation. We found a clear correlation between the bundle diameter distribution (obtained by statistical evaluation of TEM images of deposited material) and the optical absorption spectrum; the absorption peaks shift from 1.8 to 1.5 eV and from 2.7 to 2.4 eV with increasing diameter. The structure of the peaks suggest that the samples are heterogeneous, consisting of at least two phases. This is a breakthrough for nanowire wet processing, since it tremendously speeds up the characterisation of dispersions.

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ELECTRON MICROSCOPY AND XPS STUDY OF WS2 NANOPARTICLES AND NANOTUBES INTERCALATED BY ALKALI METALS

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WS2 inorganic fullerene-like nanoparticles and nanotubes were subjected to intercalation with potassium, sodium, and rubidium atoms in heated sealed ampoules. The product of the intercalation process was not pure and was composed of both intercalated and nonintercalated phases. Electron microscopy measurements of the intercalated particles showed the interlayer expansion of outer layers that was correlated with the alkali metal radius. The XPS analysis of the rubidium intercalated material showed a rise in the Fermi energy as a result of the intercalation, endowing the originally p-type nanoparticles an n-type character.

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Tunable Graphene dc Superconducting Quantum Interference Device

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Graphene exhibits unique electrical properties on account of its reduced dimensionality and „relativistic“band structure. When contacted with two superconducting electrodes, graphene can support Cooper pair transport, resulting in the well-known Josephson effect. We report here the fabrication and operation of a two junction dc superconducting quantum interference device (SQUID) formed by a single graphene sheet contacted with aluminum/palladium electrodes in the geometry of a loop. The supercurrent in this device can be modulated not only via an electrostatic gat but also by an applied magnetic field – a potentially powerful probe of electronic transport in graphene and an ultrasensitive platform for nanomagnetometry.

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Torsional Stick-Slip Behavior in WS2 Nanotubes

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The mechanical properties of WS2 Nanotubes are of great interest from both scientific and application point of view.Their perfect crystalline structure results in superior mechanical properties compared to bulk materials.Here we present measurements of torsion and shear modulus of WS2 nanotubes.A suspended nanotubepedal device clamped at the two ends was fabricated using e-beam lithography and gold evaporation.The nanotube was twisted by pressing the pedal with an AFM tip and force curves were recorded.We experimentally observed atomic scale torsional stick-slip behavior in these individual WS2 nanotubes.We found that when an external torque is applied to a WS2 nanotube,all its walls initially stick and twist together,until a critical torsion angle,at which the outer wall slips and twists around the inner walls.This is followed by a series of secondary stick-slip torque oscillations.We present a theoretical model based on DFTB calculations,which explains the torsional stick-slip behavior in terms of a competition between the effects of the in-plane shear stiffness of the WS2 walls and the inter-wall friction arising from the atomic corrugation of the interaction between WS2 walls

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ELECTRONIC AND MECHANICAL PROPERTIES OF CHEMICALLY DERIVED GRAPHENE

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The peculiar electronic properties of graphene have attracted great interest in the past few years. However the currently existing methods to obtain graphene sheets donât enable large-scale production. Thus alternative production methods are highly desirable. Here we report on the electronic and mechanical properties of single graphene sheets obtained via chemical reduction of graphite oxide.

We find that reduced single layers exhibit room temperature field effect mobility up to 1000 cm2/Vs. The structure of the sheets is best described by intact, nanometer-sized graphitic domains separated by defect clusters, which results in hopping conduction as the dominant charge-transport mechanism.

Towards their mechanical characterization we have performed AFM indentation experiments on free-standing single layers. For single layers we find a mean elastic modulus of 0.2TPa. Another interesting feature of these monolayers is that their elastic modulus scales inversely with their electrical conductivity. Furthermore, built-in tensions are found to be significantly lower compared to mechanically exfoliated graphene.

Strategies for improving sample conductivity will be also discussed.

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CVD Growth of Carbon Nanotubes Using Molecular Nanoclusters as Catalyst

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For transport measurements on Carbon Nanotubes (CNTs) and functionalized derivatives such as peapods isolated single-walled carbon nanotubes (SWNTs) are favourable. With the chemical vapour deposition (CVD) method such CNTs can be grown directly on substrates and their quality is governed by the catalyst. Our experiments are motivated by a possible constriction of the CNT diameter distribution, which could facilitate the synthesis of peapods. Hence we investigated CNTs grown with molecular $Mo_{72}Fe_{30}$ nanoclusters as a catalyst on different substrates by AFM, SEM and Raman spectroscopy. In comparison to our standard catalyst, which is composed of Fe clusters agglomerated at alumina nanoparticles, the molecular nanoclusters could enable the growth from highly defined catalyst particles. Although CNTs can be grown successfully in general, a chemical reaction of the catalyst with substrate surfaces may inhibit the growth in certain cases. Additionally a possible role of the oxidation state of Mo for the growth mechanism is discussed.

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Electronic and vibronic properties of pristine and doped graphene layers

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In realistic graphene devices, the electronic properties are modified by interlayer coupling, substrate interaction or electron-electron correlation effects. Studying stage one graphite intercalation compounds using a combined angleâresolved photoemission spectroscopy (ARPES) and theory approach is an elegant way around these problems. Our ARPES data highlight that the full experimental Dirac cone of graphene can be determined. The kink in the quasiparticle dispersion is compared to the phonons from inelastic x-ray scattering (IXS) and the energy is in good agreement to the observed Kohn anomaly for the TO phonon branch close to K point. This reflects, that electron phonon coupling can indeed be seen in both the quasiparticle and phonon dispersion relations. Based on our ARPES and IXS data we provide a new set of tight-binding (TB) parameters for efficient calculation on the quasiparticle and phonon dispersions in pristine and doped few-layer graphene and graphite including electron-electron correlations. This is the first set of TB parameters that can describe both the low and high energy properties relevant for transport and optical spectroscopy experiments, respectively.

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The Effect of Pressure on Graphene-Related Materials

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In this work we combine theoretical and experimental techniques to investigate graphene-related materials. From the theoretical point of view, we address the interplay between structural and electronic properties of graphene layers, ribbons and epitaxial graphene. We study the structural rearrangements of a crossed junction of ribbons (graphene on top of epitaxial graphene) taking into account the substrate effect. Effects of external pressure are also considered, and the change in the

electronic states are described. Similar studies are conducted for bi- and trilayer graphene under pressure. The effects of doping, particularly with Nitrogen, on the structural and electronic properties (with and without pressure) are discussed. The first-principles calculations are based on the Pseudopotential Density Functional Thoery(DFT) within the Local Density Approximation(LDA) for the exchange-correlation functional, as implemented in the SIESTA program. We propose and perform some experiments based on the application of pressure with an AFM tip on the samples, and we also perform Electrostatic Force Microscopy(EFM) images to study the structural end electronic modifications of the material.

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Group theory analysis of electrons and phonons in N-layer graphene systems

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In this work we study the symmetry properties of electrons and phonons in graphene systems as function of the number of layers. We derive the selection rules for the electron-radiation and for the electron-phonon interactions at all points in the Brillouin zone. By considering these selection rules, we address the double resonance Raman scattering process. The monolayer and bilayer graphene in the presence of an applied electric field are also discussed.

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Effects of gamma irradiation on carbon nanotubes and their composites with nanodiamond

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Across the main radiation environments including heavy ions, gamma and proton radiation, nanoscale materials may outperform their conventional counterparts, where the improvement is attributed to nanoscale functionality. While diamond is known being radiation hard, carbon nanotubes are also of great interest owing to structural (high aspect ratio) properties and apparent radiation resiliency. For âharshâ radiation environment applications, it is critical to demonstrate their structural integrity and optimal performance. We studied single- and multiwalled nanotubes and composites with nanodiamond forming truly trigonal-tetragonal nanocomposites. They were subjected to gamma irradiation of 50, 100 and 10^3 kGy and analyzed prior to and post-irradiation using various analytical tools. Although the structure and defects dynamics in carbon nanostructures remain elusive, this

investigation imparts insights into the gamma radiation induced events. It is found single-walled nanotubes improved their radiation resilience with nanodiamond and the radiation-induced microscopic defects aggregation/ amorphization, and bonding re-arrangement collectively known as Wigner effect are discussed.

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Laser beam as a simultaneous tool and an in situ probe for a CNTs growth by a Laser Assisted CVD method

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We report on a flexible and simple method for a local CNTs growth and its in situ monitoring. The method of Laser Assisted Chemical Vapor Deposition (LA CVD) uses a laser beam to heat locally the substrate. The objective is to prepare a predefined type of CNT assemblies at selected locations on the substrate while preserving the unexposed part of the substrate from a high temperature exposure. The LACVD reactor contains temperature and pressure sensors, three in situ optical detectors, a horizontal substrate holder and an optical assembly that focuses the laser beam with the wavelength of 800 nm on the substrate at a 35 deg incidence angle. One optical detector records the intensity of light reflected under 35 deg from the sample. Other two detectors monitor visible and infra red light emitted by the sample, respectively. We investigated the correlation between in situ detected optical signals and ex situ characteristics obtained from SEM and Raman spectroscopy on samples for which the growth process was stopped at different stages. The obtained information enables us to control the growth process for producing either 2D horizontal networks or 3D vertically aligned forests of CNTs

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Defect Induced Photoluminescence from Dark Excitonic States in Individual Single-Walled Carbon Nanotubes

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Most of the excitonic states formed by the strongly correlated electron-hole pairs in carbon nanotubes are non-emissive. The selection rules for one photon absorption and emission are imposed on the excitonic states by symmetry and spin conser-

vation laws. We show experimentally that these rules can be relaxed by locally perturbing the electronic structure of the nanotube. We introduced defects in the sidewalls of single nanotubes by intense pulsed laser excitation and observed modified photoluminescence (PL) spectrum with new low energy emission bands [1]. Satellite peaks for different (6,4) and (5,4) nanotubes have redshifts of 30-60 meV, attributed to the ${}_0A_0^+$ states, and 110-190 meV. These PL bands with large energy separation also emerge after the treatment of the nanotubes with aqueous solution of gold. We assign this emission to the triplet state where the spin polarized states induced by the defect creation or metal adatoms facilitate the intersystem crossing. The triplet state has up to two orders of magnitude longer lifetime (∼170ps) than the bright singlet exciton.

[1] H. Harutyunyan et al., arXiv:0812.1040v1.

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Quantitative composition of a single-walled carbon nanotube sample: Raman scattering vs. Photoluminescence

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The growth processes of Carbon Nanotubes (CNTs) yield samples containing tubes with a large variety of different chiralities. The qualitative composition of the CNTs product has been revealed by Raman scattering [1] and by Photoluminescence Emission (PLE) [2]. The quantitative composition remains a task in CNT characterization. We adress this problem by comparing the relative PLE intensities of a subset of semiconducting nanotubes with the relative intensities of the according Radial Breathing Modes obtained by Raman scattering. The PLE measurements were performed by dissolving the HiPCO grown nanotubes in aqueous solution using sodium dodecylbenzene sulfonate as surfactant. Raman Spectroscopy was performed by depositing the tubes from the solution on a silicon substrate by spin-coating. The presence of the CNTs was confirmed by atomic force microscopy. We show that the two methods yield significantly different ratios. Correcting these ratios by theoretical predictions of the processes involved, we confirm by both the methods that one carbon nanotube species dominates the population.

[1] J. Maultzsch et al., Phys Rev B. 2005
[2] S.M. Bachilo et al., Science, 2002

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The Role of Bundles in Separating Metallic from Semiconducting Single Walled Carbon Nanotubes via Density Gradient Centrifugation and Electrophoresis

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Separating SWNTs by electronic type has become a flourishing research field and enrichment of m-SWNTs has been achieved by various techniques including dielectrophoresis and density gradient centrifugation (DGC). All such separation methods make use of liquid suspensions, typically of individualized and isolated tubes in water. Many studies have used surfactants, such as sodium dodecyl sulfate (SDS), sodium dodecylbenzene sulfonate (SDBS) or sodium cholate (SCho) to disperse SWNTs and the yield of individualized tubes depends on the combination of starting raw SWNT material, surfactant, ratio of surfactant to SWNTs starting concentration and centrifugation conditions. In the current work we demonstrate that by controlled aggregation of s-SWNTs in suspension it is possible to separate m- from s-SWNTs either by DGC due to differences in densities or by gel electrophoresis (EP) due to differences in bundle sizes. Due to the sonication conditions used in this work m-SWNTs are preferentially suspended to individuals and s-SWNTs remain in bundles. Evidence is provided by optical absorbance spectroscopy and atomic force microscopy (AFM).

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Combined Electronic Transport and Raman Measurements on Individual Single-Wall CNTs

Olli Herranen[1] Jyri Rintala[2] Andreas Johansson[1] Mika Petterson[2] Markus Ahlskog[1]
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Single-wall carbon nanotubes (SWCNT) are very good candidates for future nanoscale circuitry because of their unique electronic properties. Therefore it is important to investigate their properties. We have performed both Raman and electronic transport measurements on individual single-wall carbon nanotubes over a relatively broad diameter range (0.8-2.7 nm). Single nanotube devices were made on top of a highly doped Si wafer covered with 300 nm thick SiO_2. The Si wafer was used as a backgate and the ends of the CNTs were connected by electrodes of Pd. Raman measurements were performed using either a 632.8 nm or a 532 nm laser as the excitation source. From the G-band in the Raman spectra we could determine if the tubes are metallic or semiconducting, and when the RBM mode was visible, it gave us a way to deduce the chiral indices of the tubes. The electronic structure of the same nanotubes was further probed by transport measurements made at cryogenic temperatures. From the measurements we could e.g. estimate the band gap of the semiconducting nanotubes. The transport and Raman measurements where consistent and confirmed each other in all cases.

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Graphene II and theory of carbon nanotubes

8:30 – 9:00	J. Hone, US *Graphene mechanics, tribology, Raman spectra under strain, and NEMS.*
9:00 – 9:30	K. Kern, DE *Doping effects in pristine and epitaxial graphene*
9:30 – 10:00	J. C. Meyer, DE *Microscopic studies of graphene*
10:00 – 10:30	Coffee break
10:30 – 11:00	T. F. Heinz, US *Optical spectroscopy of single and few-layer graphene*
11:00 – 11:30	E. Andrei, US *Scanning tunneling spectroscopy and transport measurements in suspended graphene*
11:30 – 12:00	A. C. Ferrari, UK *Raman spectroscopy of graphene under uniaxial strain*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	M. Damnjanović, RS *Classification and diffraction of quasi one-dimensional crystals*
19:00 – 19:30	C. Ambrosch-Draxl, AT *NaPhoD - nano-hybrids for photonic devices*
19:30 – 20:00	S. A. Maksimenko, BY *Electrodynamics of carbon nanotubes: principles, device applications and open questions*
20:00 – 21:00	Poster Session II – TUE

Tuesday, March 10

8:30

Graphene mechanics, tribology, Raman spectra under strain, and NEMS.

James Hone[1] Changgu Lee[1] Xiaoding Wei[1] Mingyuan Huang[1] Hugen Yan[1] Sami Rosenblatt[1] Changyao Chen[1] Kirill Bolotin[1] Jeffrey Kysar[1] Horst Stormer[1] Tony F. Heinz[1]
[1]Columbia University, New York

This talk will discuss recent experimental results in four areas related to the mechanics of graphene. First, we have used AFM nanoindentation to measure the elastic modulus and ultimate strength of graphene films. The data show graphene to be the strongest material ever measured, with an ultimate strain level near 25 percent; the nonlinear elasticity matches well with theoretcal models. Second, the measured frictional properties of graphene show a strong dependence on the number of layers, and reveal the atomic lattice orientation. Third, measurements of the Raman spectrum of graphene under uniaxial strain reveal pronounced redshifts, and a splitting of the G mode that is related to the breaking of the symmetry of the graphene lattice. Fourth, we have fabricated graphene NEMS resonators, and used an electromechanical mixing technique to read out their motion. The devices show robust signals, and pronounced shifts in response to mass loading.

9:00

Doping effects in pristine and epitaxial graphene

Klaus Kern
Max-Planck-Institut für Festkörperforschung, Stuttgart and Ecole Polytechnique Fédérale de Lausanne

Graphene is emerging to be an important electronic material due to a number of interesting physical properties â such as strict two-dimensionality, peculiar bandstructure and high carrier mobility â making it highly promising for a variety of applications. Towards this goal, it is important to have a clear understanding of the electronic properties of graphene. Especially, the microscopic understanding of metal-graphene contacts is vital for the successful realization of novel devices.

We have studied the electronic structure of pristine and epitaxial graphene and the effect of metal contacts by integral and local methods. Using low-temperature scanning tunneling microscopy we were able to characterize the quasipaticle chirality in epitaxial graphene. Upon deposition of metals we observe a significant charge transfer, changing the local electronic structure. The charge transfer at metal-graphene interfaces is further studied by scanning photocurrent microscopy and angle-resolved photoemission spectroscopy. From these experiments guidelines for the tuning of the electronic properties of graphene by the right choice of metal can be drawn.

9:30

Microscopic studies of graphene

J. C. Meyer[1] A. Chuvilin[1] G. Algara-Siller[1] S. Kurasch[1] J. Biskupek[1] U. Kaiser[1] C. O. Girit[2] M. Crommie[2] A. Zettl[2] C. Kisielowski[3] R. Erni[3] M. D. Rossell[3]
[1]Materialwissenschaftliche Elektronenmikroskopie, Universität Ulm, Ulm
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Freely suspended mono-layer graphene is the thinnest possible membrane that is conceivable with currently known materials. Yet, it is remarkably stable under high-energy electron irradiation and thus opens unprecedented opportunities for electron microscopic studies. On the one hand, the graphene membrane structure and its defects are of outstanding interest for science and applications of this promising new material. Static deformations, topological defects, various vacancy configurations or dislocations are detected by transmission electron microscopy (TEM). On the other hand, graphene membranes can serve as a perfect sample support for transmission electron microscopy. Its contribution to the TEM image signal can be filtered out completely and adsorbed atoms and molecules on the graphene sheet can be imaged as if they were suspended in free space. The synthesis, applications and numerous examples of conventional and aberration-corrected electron microscopic results are presented. As an outlook, the use of atomically thin membranes for lowest-voltage electron microscopy and challenges and promises in using graphene as a molecular support are briefly discussed.

10:30

Optical spectroscopy of single and few-layer graphene

Tony F. Heinz
Department of Physics, Columbia University, New York USA

Optical spectroscopy provides a powerful tool to probe the structure and dynamics of electronic excitations in graphene. As the most basic measurement, we have characterized the optical absorption of single-layer graphene. Like the Manchester group, we find a spectrally flat absorbance from 0.5 eV to the visible, with a magnitude of $\pi\alpha = 2.3\%$, where α is the fine structure constant. At lower photon energies, however, we see departure from this universal behavior associated with the effect of finite carrier concentration. Analogous results have been obtained for few-layer graphene samples. With increasing layer number, we observe the onset of new interband transitions. We can describe these results in terms of the folded 3D graphite band structure.

Femtosecond spectroscopy permits probing the dynamics of these excitations. After creation of electron-hole pairs, equilibration of the carriers among themselves and with strongly-coupled optical phonons occurs on a sub-picosecond time scale, while full thermalization develops on the picosecond time scale. On a still slower time scale, we can characterize the heat flow into the substrate.

11:00

Scanning tunneling spectroscopy and transport measurements in suspended graphene

Eva Andrei
Rutgers University

The recent discovery of methods to isolate graphene (a one-atom thick layer of crystalline carbon) has opened an extraordinary arena for new physics and applications stemming from charge carriers that are governed by quantum-relativistic dynamics. Because of the 2-dimensinal nature of graphene the properties of its relativistic charge carriers are easily obscured by environmental disturbances such as potential fluctuations induced by insulating substrates. I will describe scanning tunneling spectroscopy[1,3] and transport[2,4] experiments on suspended graphene samples which are decoupled from substrate fluctuations. Our findings include direct observation of the Landau levels, measurement of the Fermi velocity, and evidence for electron-phonon and electron-electron interactions. In addition we find that, in contrast to non-suspended samples, the suspended samples show Quantum Hall plateaus associated with interactions leading to valley-splitting appearing already at very low fields.

1.G. Li , E.Y. Andrei - Nature Physics,3, 623 (2007)
2.X. Du, G. Li, A. Barker, E. Y. Andrei, Nature Nanotecnology 3, 491 (2008)
3. G. Li, A. Luican, E. Y. Andrei arXiv:0803.4016
4.X. Du, I. Skachko, E.Y. Andrei, PRB 77,184507 (2008)

11:30
Raman spectroscopy of graphene under uniaxial strain

Andrea C Ferrari[1] T. M. G. Mohiuddin[2] A. Lombardo[1] R. R. Nair[2] A. Bonetti[1] G. Savini[1] R. Jalil[2] N. Bonini[3] D. M. Basko[4] C. Galiotis[5] N. Marzari[3] K. S. Novoselov[2] A. K. Geim[2]
[1]Engineering Department, University of Cambridge, Cambridge
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[4]Laboratoire de Physique et Modelisation des Mileux Condenses, Universite Joseph Fourier and CNRS, Grenoble, France
[5]FORTH ICEHT and Materials Science Dept., University of Patras, Patras, Greece

Raman spectroscopy is a powerful tool for graphene characterisation [1] Here we show the effects of uniaxial strain [2]. The E2g mode splits in two, one polarized along the strain and the other perpendicular. This splits the G peak in G+ and G-, similar to curvature for the nanotube G peak. Their intensities depend on light polarization, allowing the determination of the graphene crystallographic orientation [2]. We study the Gruneisen parameters for the G, D and Dâ peaks [2]. These allow us to reconcile previous experiments on graphite and carbon fibres, and are the starting point to understand the effects of strain on nanotube phonons. We then discuss how discriminate the effects of strain on the Raman spectrum from disorder and doping [3-5]. We also show how the D peak probes gap opening in chemically modified graphene [6], and present evidence of photoluminescence in nanostructured graphene.

1 A. C. Ferrari et al Phys. Rev. Lett. 97 187401 (2006)
2 T. M. G. Mohiuddin et al arXiv:0812.1538
3 S. Pisana et al. Nature Mat 6 198 (2007)
4 A. Das et al Nature Nano 3 210 (2008)
5 C. Casiraghi et al. Appl. Phys Lett. 91 233108 (2007)
6 Elias et al. arXiv:0810.4706

18:30
Classification and diffraction of quasi one-dimensional crystals

Milan Damnjanović[1] Tatjana Vuković[1] Ivanka Milosević[1]
[1]University of Belgrade, Belgrade

There are fifteen elementary conformation classes out of which any regular (i.e. helically periodic) quasi one dimensional structure, like nanotube or stereoregular polymer is built. For each of them the full symmetry, described by one of the line groups, is determined and used to find the diffraction intensity distribution within kinematical model. It is shown that the diffraction intensity distribution is a product of the atomic scattering amplitude (comprising the physical information on the type of the system) and the geometrical factor, which is easy to calculate form the full symmetry.

The possible diffraction patterns are discussed, and their features are analyzed in order to be able to determine the structure of any quasi one dimensional system by diffraction. In particular, single wall carbon nanotubes themselves are the elementary systems (belonging to different conformation classes depending on their chirality). It is shown that the obtained results enable unique characterization of carbon nanotubes by diffraction measurements.

19:00

NaPhoD -â nano-hybrids for photonic devices

Claudia Ambrosch-Draxl
Chair of Atomistic Modelling and Design of Materials, University of Leoben, Leoben

Nano-hybrid systems composed of a photoactive organic molecule (pea) inside the cage of a single wall carbon nanotube (pod) represent the realization of new nanosize photonic devices with tunable emission. Conjugated rigid rod molecules are widely studied for their optical properties. Due to their size they are suitable for the inclusion in SWNTs, being optimal candidates for emitting in the visible spectral range. Such peapods have been synthesized and characterized using experimental and theoretical techniques. As an example, oligothiophenes were encapsulated by means of low-pressure gas-phase manipulation. The presence of the pea inside the carbon cage was proven by Raman spectroscopy, while transmission electron microscopy images confirmed their endohedral position and acquired information on their relative orientation with respect to the nanotube walls. First-principles calculations based on density functional theory could reveal the optimal diameter of the tube for the encapsulation, the orientation of the molecule inside the tube, as well as the binding energies. The ab-initio approaches also allow for an analysis of the peapods' electronic structure and optical properties.

19:30

Electrodynamics of carbon nanotubes: principles, device applications and open questions

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A research discipline â nanoelectromagnetics â is introduced as a synthesis of macroscopic electrodynamics and microscopic theory of electronic properties of different nanostructures exemplified by carbon nanotubes (CNTs). A strong slowing down of surface waves is demonstrated and the concept of nanotube as a nanowaveguide in the IR and THz ranges is introduced. An analysis of the scattering pattern and the absorption cross-section of finite-length CNTs and CNT bundles is presented. Comparison with experimental results is carried out allowing physical interpretation of low-frequency absorption band observed in experiments. Potentiality of CNTs as interconnectors is demonstrated. Antenna properties of CNTs are described and the thermal radiation of isolated CNT is shown to be clearly nonmonotonous allowing the thermal antenna concept. Strong local field enhancement is predicted to be inherent to metallic CNTs in the near-field zone providing necessary mechanism for far-IR and THz near-field optics. The idea of CNT as molecular analog of FEL is proposed and discussed. The problem of spontaneous radiation of an excited atom in CNT is considered as a possible mechanism of CNT antenna excitation. Prospective problems of electrodynamics of CNTs are formulated and discussed.

1
Aharonov-Bohm effect in a side-gated graphene ring

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Over the last years graphene has received a lot of attention in both theory and experimental research. Although there are many publications dealing with constrictions and dots in a broad variety, little research has been done on graphene rings.

We present four-terminal magnetoresistance measurements on a side-gated ring structure etched out of a single-layer graphene flake. Aharonov-Bohm oscillations are observed in both the two- and the four-terminal resistances. The best visibilities are around 13%.

Furthermore the traces are in accordance with the Onsager theorem showing $G(B) = G(-B)$ symmetry. The ring radius derived from the oscillation period agrees with the average geometric radius of the ring of 275nm.

By changing the voltage applied to the side gates, we are able to change the relative phases of the two alternative paths, and induce phase jumps of π. The same effect can be obtained by changing the applied back gate voltage. The voltage changes needed on the gates to introduce such phase jumps are consistent with the relative lever arms of the gates.

2
Dispersion of Single Walled Carbon Nanotubes using Synthetic Oligonucleotides

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Both synthetic oligonucleotides and natural ds-DNA have been shown to be effective at dispersing single walled carbon nanotubes (SWNTs) in water.In this study, HiPCO SWNTs were dispersed in H2O using dA15, dT15, dC15 and dG15,and the solutions were monitored over several weeks using absorption, near-IR photoluminescence (NIR-PL) and circular dichroism (CD) spectroscopy, atomic force microscopy (AFM),and zeta potential in order to compare experimentally obtained dispersion efficiencies to those calculated theoretically.In line with theoretical predictions, the pyrimidines displayed greater dispersion efficiency than the purines,with the dT15 performing strongest in terms of debundling and wrapping,whereas the dA15/SWNT solution was observed to re-aggregate over time, perhaps due to self-stacking of the base in solution.Also, as previously seen for dispersions of SWNT in ds-DNA, quenching of the PL is initially observed and reappears over a number of days: the rate at which the PL reappears and its subsequent intensity are direct indicators of the dispersion efficiency; these results are borne out by spectroscopic analysis and by the mean diameters of the SWNT/DNA hybrids over time.

3

Effects of ion beam heating on Raman spectra of single-walled carbon nanotubes

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Free standing films of single-wall carbon nanotubes were irradiated with energetic N^+ and C^{4+} ions. The observed changes in the Raman line shape of the radial breathing mode and the G band of the C^{4+} irradiated samples were similar to those found for a thermally annealed sample. We ascribe these changes to thermal desorption of volatile dopants from the initially doped nanotubes. A simple geometry of the experiment allows us to estimate the temperature rise by one-dimensional heat conductance equation. The calculation indicates that irradiation-mediated increase in temperature may account for the observed Raman spectra changes.

4

Electron spin properties of La@C_{82} in empty fullerene matrices

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Mono-metallofullenes M@C_{82} have attractive magnetic properties which can be applied to quantum information processing. Furthermore, M@C_{82} molecules have great potential as building blocks for solid state quantum nanodevices. The ESR spectrum of a radical electron on C_{82} cage of La@C_{82} in solution can be identified by its hyperfine interaction with $I = 7/2$ of ^{141}La. The hyperfine structure (hfs) of solid La@C_{82} has not been reported because of the exchange and spin-spin interactions between La@C_{82} molecules. Here, we report the concentration dependent ESR properties and hfs of La@C_{82} diluted in various empty fullerene matrices. The ESR data suggest that the intermolecular dipole-dipole interaction between La@C_{82} molecules can be controlled by changing the concentration of La@C_{82}, and furthermore that $C_{82}(C_2(3))$ is the best matrix to disperse La@C_{82}. The dispersion ability of empty fullerene matrices depends on the cage size of empty fullerenes. La@C_{82} is especially difficult to disperse in a C_{60} matrix because of the large difference in cage size.

5

Investigation of N@C_{60} and N@C_{70} stability under high pressure and high temperature conditions

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Endohedral fullerenes encapsulating single nitrogen atoms (N@C_{60} and N@C_{70}) are spin active, with exceptionally long electronic spin coherence times. Due to the high reactivity of nitrogen, the stability of these molecules at elevated temperatures is poor, drastically restricting the possibilities for chemical treatment. In the first part of this study, N@C_{60} and N@C_{70} in toluene solutions were subjected to high pressure up to 0.8 GPa at room temperature and annealed for 1, 2 or 24 hours. In the second part of the study, high pressure was complemented by elevated temperatures. In each case the number of surviving molecules was evaluated comparing spin counts of *ex*-situ electron paramagnetic resonance (EPR) spectra before and after the treatment. The stability of N@C_{60} and N@C_{70} under high pressure and high temperature conditions is discussed in comparison to previous studies under normal pressure.

6

1D supramolecular aggregates of PAHs and 2D assemblies of phenylene-ethynylene-macrocycles on HOPG

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Small polyaromatic systems, such as dibenzonaphthacenes, may be thought as small models for graphenes. Dibenzonaphthacenes were functionalized with linear phenylene-ethynylene oligomers, terminated with long alkyl chains to improve the solubility in organic solvents. We have shown by means of AFM, that such systems may form pi-stacked supramolecular aggregates under appropriate solvent conditions. These systems are models for molecular organic nanowires based on stacked PAHs.

Phenylene-ethynylene-macrocycles are shape-persistent, ring-like molecular building blocks for the formation of well defined two dimensional molecular networks on flat surfaces. Such self-assembled physisorbed adlayers can be used as crystalline, well arranged templates for the deposition of small guest molecules in their interior, e.g. fullerenes or gold nanoparticles, or may be further functionalized to achieve self sorting surfaces. The morphology is determined by the ring diameter, and its extra annular functionalization, e.g. by alkyl chains. Phenylene-ethynylene-macrocycles were synthesized, and their monolayers on HOPG were investigated by STM.

7

Resistance Fluctuations in Graphene

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We have measured resistance fluctuations that persist at temperatures up 50 K in graphene monolayer samples deposited on a Si/SiO2 substrate. The decrease of the amplitude of the fluctuations as temperature increases is qualitatively well described by inverse power laws similar to those seen for the temperature dependence of universal conductance fluctuations (UCFs) in disordered metals and explained by the Lee-Stone-Fukuyama theory. However, the much higher temperatures at which the fluctuations are seen suggests a significant difference, and the behaviour of the amplitude as the gate voltage varies appears to provide a challenge for current theory.

8

The reaction of lithium metal vapor with carbon nanostructures

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Raman spectroscopy and in-situ Raman spectroelectrochemistry were applied to study the products of the reaction of lithium metal with carbon nanostructures: single walled carbon nanotubes (SWCNT) and fullerene peapods (C60@SWCNT). In general, a strong degree of doping was proved by the vanishing of the SWCNTâs radial breathing mode (RBM) and by the attenuation of the tangential (TG) modes intensity by two orders of magnitude. For C60@SWCNT the reaction with Li metal vapor caused a frequency downshift of the Ag(2) mode of the intratubular C60 by 27 cm-1 and changed the resonance condition of encapsulated fullerene. In contrast to potassium vapor doping, the strong downshift of the frequency of the TG band has not been found for Li-doping. The carbon nanostructures after reaction with Li metal vapor were exposed to humid air and examined by Raman spectroscopy. The residual Li doping even after water treatment has been confirmed for C60@SWCNT by in-situ Raman spectroelectrochemical measurements. The TG mode of the Li doped peapods does not upshift during the anodic doping, which points to the formation of a stable exohedral metallofullerene peapod.

9
Study on cellular adhesion of human osteoblasts on nano-structured diamond films

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The need of new biocompatible materials with superior properties and flexibility in their surface termination and functionalization for medical applications is constantly increasing. Due to combination of intrinsic properties, chemically deposited diamond thin films are proposed as one of the most promising material in this field. They are chemically/mechanically/physically stable and their surface can be modified by variety of chemical or plasmatic techniques. We present the impact of diamond nano-morphology on of human osteoblasts. Different NCD nano-patterns, i.e. nanorods, cauliflower-like structures and irregular nanostructures, were prepared by plasma etching process applying various masking materials (Ni, Au and NCD powder). We observed that attachment of osteoblasts is guided by the NCD nanostructure as visualized by scanning electron microscopy and fluorescence microscopy. Few but large focal adhesions are formed on irregular nanostructures and many but very fine ones are formed on nanorods and cauliflower-like structures. We suggest that the cell adhesion is controlled by nano-structured films thereupon their usage in bio-medical applications could be considered.

10
Surface attenuated infrared absorption in hybrid materials of conducting polymers and carbon nanotubes

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We will present infrared spectra of carbon nanotubes wrapped by conducting polymers polyaniline, polycarbazole and melanin. These hybrid materials have been prepared by electrochemical polymerization and exhibit increased conductivity and enhanced electron transfer from the electrolyte to the electrode. Infrared spectra of similar systems show the so-called surface-attenuated infrared absorption (SAIRA) effect:[1] interaction of the polymers with the nanotube surface results in attenuation of in-plane vibrations while the out-of-plane vibrations are not affected. The magnitude of the attenuation depends on the strength of the nanotube-polymer interaction, i.e. the contact between the evanescent field of the nanotube surface

and the wrapping polymer. We compared the spectra of the hybrids and found the most outspoken effect in the case of polyaniline, in accordance with the results of UV-VIS and impedance spectroscopy.

[1] K. Setyowati, M.J. Piao, J. Chen, H. Liu: *Appl. Phys. Lett.* **92**, 043105 (2008).

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11

Characterization of Commercially Available Singlewall and Multiwall Carbon Nanotubes

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Laser Ablation Singlewall Carbon Nanotubes from SINEUROP-Nanotech GmbH and various CVD grown multiwall carbon nanotubes (Ahwahnee Raw Multiwall Carbon Nanotubes, Arkema GraphistrenghtC100, BaytubesC150P, CTube and Nanocyl 7000 Multiwall Carbon Nanotubes) were characterized by atomic force microscopy, scanning electron microscopy, Raman spectroscopy, and X-ray diffraction. These data were correlated with the electrical conductivity obtained by the four-lead technique on bucky paper or filter cake as well as with conductivity data from compressed powders. The conductivity of as-grown Laser Ablation Singlewall tubes varies between 710 and 170 S/cm, respectively, depending from what part of the reactor the samples are collected. The highest conductivity of multiwall tubes was found on NanocylÂ®7000 and amounted to 85 S/cm. Implications for various industrial applications of carbon nanotubes will be discussed.

12

Dry manufacturing of SWCNT-based flexible, transparent conducting electrodes

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Thin films of single-walled carbon nanotubes (SWCNTs) are considered to be strong candidates for ITO replacement as flexible, transparent conducting electrodes (TCE) for e.g. flexible displays. We have developed a dry, direct method for the preparation of SWCNT films. SWCNTs were synthesised by an aerosol method ba-

sed on the ferrocene vapour decomposition in CO atmosphere and collected directly from the gas phase via the filtering nitrocellulose filters. A thermo-compression method was adapted for transferring the SWCNT layers to PET films. We studied the effect of reactor the temperature as well as the residence time on the SWCNT characteristics and TCE film properties. When increasing the nanotube length and reducing the bundle diameters, we produced flexible TCEs having 50 ohms/sq sheet resistance at 80 % transmittance with 550 nm photons, after briefly treating the films with a drop of nitric acid. These TCE offer an alternative to replace ITO as TCE e.g. in flexible active matrix OLED displays.

13

Supramolecular assembly of SWNT and Ru(II)-bipyridine complex: Coupling of the organometallic redox functions with nanotube doping

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The amphiphilic Ru-bipyridine complex, NaRu(4-carboxylic acid-4'-carboxylate-2, 2'bipyridine) (4,4'-dinonyl-2,2'bipyridine)(NCS)2 can be used as a surfactant for solubilization of single walled carbon nanotubes (SWNTs) in acetonitrile-t-butanol mixture. Electrochemical n-/p-doping of a supramolecular assembly was studied for the first time by in-situ Raman spectroelectrochemistry. Whereas the Raman lines assigned to the nanotube (RBM and G-bands) attenuate their intensities upon both n- and p-doping, the Raman lines, assigned to the bipyridine ring vibrations, selectively attenuate for the p-doping only. The explanation is based on the erasing of resonance enhancement in a doped supramolecular assembly. Whereas the charge transfer localized on the Van Hove singularities is generally amphoteric, the charge transfer localized on the Ru(II)-bipyridine is not. The p-doping of the Z-907Na/SWNT assembly at potentials positive to ca. 0.7 V vs. Ag-pseudoreference causes faradaic oxidation of Ru(II) to Ru(III), but there is no mirror effect (reduction of Ru(II)) upon n-doping at the used potentials, by -1.6 V vs. Ag-pseudoreference.

14

The morphology of Silicon nanowire samples: A Raman study

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Raman spectra of silicon nanowires (SiNWs) are studied as a function of laser excitation power and temperature. With increasing temperature and laser excitation power a typical red-shift of the SiNWs first order optical mode is obtained. At ambient conditions, the power dependent Raman shift shows a saturated behavior beyond a critical power. Similar measurements, under vacuum, rule out effects due

to thermal convection as a reason for the observed Raman shift saturation. The irreversibility of the power-dependent Raman shifts and the reversibility of temperature dependent shift suggest that the observed saturation of the frequency shift can be explained with a change in sample morphology. Finally, a simulation of the SiNW Raman spectra reveals that the temperature behavior can be explained by a four phonon anharmonic process.

15

Reduction-Controlled Viologen in Bisolvent as an Environmentally Stable n-Type Dopant for Carbon Nanotubes

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Various viologens have been used to control the doping of single-walled carbon nanotubes (SWCNTs) via direct redox reactions. A new method of extracting neutral viologen (V0) was introduced using a biphase of toluene and viologen-dissolved water. A reductant of sodium borohydride transferred positively charged viologen (V2+) into V0, where the reduced V0 was separated into toluene with high separation yield. This separated V0 solution was dropped on carbon nanotube transistors to investigate the doping effect of CNTs. With a viologen concentration of 3 mM, all the p-type CNT transistors were converted to n-type with improved on/off ratios. This was achieved by donating electrons spontaneously to CNTs from neutral V0, leaving energetically stable V2+ on the nanotube surface again. The doped CNTs were stable in water by the presence of hydrophobic V0 at the outermost CNT transistors, which may act as a protecting layer to prevent further oxidation from water.

16

Electromechanical Self-sustained Oscillations of Nanosized Field Emitters

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Carbon nanotubes (CNTs) are known to have outstanding field emission (FE) properties suitable for production of cathodes for vacuum electronic devices. Comparing to the other electron sources CNT have peculiarities of FE which are crucial for applications but their origination remains unclear till now (anomalous FE current noise, „blinking“of the electron density pattern, unexpected trajectories of electrons). At the same time there are observations of the „strange“mechanical oscillations of single CNT driven by a DC voltage. Here we present results of experimental and theoretical studies of FE from nanomaterials. In case if the cathodes are flexible, we observed the mechanical and FE current KHz oscillations driven by a DC voltage. To explain the oscillations we propose a model of the emitter as a mechanical oscillator in the electric field. Computer simulation shows an ability of initiation of the self-sustained oscillation at certain parameters. For a single nanoemitter our model predicts the oscillations with GHz frequencies. This phenomenon opens a possibility for DC voltage conversion into GHz electromagnetic oscillations by using flexible nano-emitters.

17

Junctions of left- and right-handed chiral carbon nanotubes – nanobamboo

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The outer tube of a peapod serves as a long straight reaction room for forming of the inner tube by coelascing of the fullerene molecules. For a given outer tube only a few types of inner tubes are allowed by the van der Waals distance. However it is possible that inner tubes with different chiralities - or the same chirality but left- and right-handedness - can start to grow in different places at the same time. A straight junction occurs at the connection of these two tubes. The geometry of different kinds of junctions containing pentagon and heptagon defects was optimized by density functional theory. The effect of the localized states on the electronic band structure was investigated.

18

Electronic structures of impurity doped carbon nanotubes

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For the electronic transport properties of semiconductors, impurities play a significant role. In carbon nanotubes, however, the effect of the impurities has not been well understood. In this paper, to clarify the properties of the impurities in carbon nanotubes, we study the electronic structures of boron or nitrogen doped carbon nanotubes using the density functional theory. We first obtain the optimized structures and discuss the stabilities of substitutional boron or nitrogen impurities. Then, we calculate the doping rate dependence of the gap of doped carbon nanotubes. From the extrapolation of the gap to the low-density limit, we estimate the depth of the impurity level. The difference between boron-doping and nitrogen-doping as well as the tube-diameter dependences of impurity states are discussed.

19

Raman signatures of WS2 nanomaterials

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Fullerene-like WS2 nanoparticles and WS2 nanotubes are studied by wavelength dependent Raman spectroscopy. The response from the nanomaterials is compared to that of 2H-WS2 crystals and microcrystalline 2H-WS2 powder. The Raman signatures point to a hexagonal 2H stacking of the WS2 layers in all nanostructures. While the wave numbers of 1st and 2nd order Raman scattering show only little dependence, the line widths and the intensity ratios exhibit a systematic evolution with respect to the specific WS2 nanostructure. The sulfur-sulfur stretching mode range is particularly sensitive to the different stages of disorder and is suitable for the diagnostic classification of the WS2 nanostructures. Raman mapping across the nanoparticles is used to distinguish between disorder and surface effects on the vibrational spectra. All the experiments were performed at low laser power, since the transformation into WO3 is induced already at moderate illumination due to the limited photo- and thermal stability of the materials.

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Core-Shell PbI2@WS2 Inorganic Nanotubes from Capillary Wetting

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One of the defining structural features of nanotubular structures is their long inner hollow cavity. Capillarity has been shown to drive the wetting and filling of carbon nanotubes with liquid and molten-phase inorganic salts. Encapsulation in the narrow void of carbon nanotubes was shown to result in a profound change of the structural chemistry of the included material relative to its bulk form. Here we demonstrate a new synthetic strategy allowing formation of core-shell nanotubular structures using multi-walled WS2 nanotubes as host templates. The relatively lar-

ge diameter of the WS2 nanotube (with inner and outer diameters of ca. 10 and 20 nm, respectively), allows a conformal folding of the guest PbI2 layers on thir interior wall, leading thus to defect-free core-shell nanotubular structures, not previously observed in carbon nanotubes[1]. Recently, new core-shell inorganic nanotubes have been prepared from compounds other than PbI2.

1. Kreizman R. et. Al., Ang. Chem. Int. Ed., In press.

21

Role of polymers in CVD growth of nanocrystalline diamond films on foreign substrates

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A growth of nanocrystalline diamond thin films becomes nowadays a routine in labs and companies over world. However, the growth of (ultra) thin films (less than 100nm) is still a technological challenge because of low nucleation efficiency on non-diamond substrates. In this work, we present an implementation of polymer based composite as the diamond nucleation layer suitable for arbitrary substrates (silicon, glass, polymer). We show that a polymer-based composite layer consisting of detonation diamond nanoparticles enhances the diamond nucleation and enables a formation of continuous nanocrystalline diamond films. This type of nucleation is well suitable for large areas and flat substrates. Using a primary polymer used as a passivation layer during standard ultrasonic seeding enables achieving good diamond growth on structured substrates. A proper combination of polymer composites with a lithographic processing is an effective way to directly growth microscopic diamond patterns on arbitrary substrates. We demonstrate electronic devices (field-effect transistors) as well as biological templates grown in this way.

22

Electromagnetic shielding properties of MWNT/PMMA composites in Ka-band

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In this work we investigated electrophysical properties of multiwall carbon nanotubes/polymethyl methacrylate (MWNT/PMMA) composites, which were prepared via coagulation technique using ultrasonic dispersion of MWNT in PMMA/NMP-DMF solution. MWNT content was varied in range 0.25-10 wt.percent. MWNT distribution in polymer matrix was controlled using optical, scanning and transmis-

sion electron microscopy. MWNT/PMMA composites, starting from small MWNT content, display high shielding efficiency (SE). Maximal attenuation was observed for composites with high MWNT content, with the value near 22-30 dB, corresponding to approximately 0.3-0.6 percent of incident radiation transfer through composite film with thickness 0.5-0.6 mm. Strong increase in SE occurs for MWNT content higher than 1 wt.percent, correlating with the percolation threshold of electrical conductivity. This phenomenon may be related with formation of long-range connectivity of MWNT network in PMMA matrix. Thus produced materials show high SE in millimeter wavelengths and may have high potential for use as components of various electronic devices due to their light weight, scalable technology and tailored properties.

23

Theoretical study of doped fullerene-cubane cocrystals

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We present a first principles study of the electronic band structure of doped fullerene-cubane ($C_{60}C_8H_8$) cocrystals using density functional theory at the local density approximation level. Three high symmetry orientations of the fullerene molecules were considered. The calculated electronic bands of the fullerene-cubane cocrystal are narrower than those of the pristine fullerene, indicating a higher superconducting critical temperature in the doped cocrystal. However, the charge transfer turned out to be incomplete [1] thus acting in the opposite way. Different oxidation state of the fullerene molecules can be achieved by doping with various alkali (K, Na) and alkali earth (Ba, Ca) atoms.

[1] V.Zólyomi, J.Koltai, J.Kürti and S.Pekker, Phys. Rev. B78, 115405 (2008)

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Raman investigation of of colloidal II-VI semiconductor heterostructures

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Colloidal nanocrystals (NCs) of II-IV semiconductor materials posses unique optical and electronic properties that offer a huge potential for applications. The NCs can be epitaxially covered with a graded shell of another semiconductor or combined into heterostructures like tetrapods. The lattice mismatch between the components introduces strain into the lattice of the initial NC core. This has a significant influences on the electronic and optical properties. We present Raman measurements of different sized nanorods with shells and tetrapods consisting of quantum dot cores as seeds and nanorod arms. Both in different combinations of CdSe, CdTe and ZnS. The influence of the additional component on the core NC is discussed, especially strain, the vibrational properties and couplings between phonons and electronic excitations.

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Electronic structure of nanotube networks

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The electronic properties of carbon nanotubes are usually obtained with the help of the zone folding method, which is based on the graphene electronic structure. During the rolling up of the graphene there are changes, however, in the angles and distances between the carbon atoms of the hexagonal network. Thus in more sophisticated calculations curvature effects and the corresponding hybridizations must be taken into account. The case is more complicated if we study nanotube networks where the rolling up method can not be used. In this case the Pi-Orbital-Axys-Vector analysis (POAV) gives some insights into the degree of hybridization. In this work we present a simple one orbital one site Hamiltonian for the study of the electronic structure of distorted nanotubes and nanotube networks. The hybridization and the effect of the non-hexagonal polygons is included in the parametrization of the method. We shall also discuss the applicability of the POAV analysis.

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ELECTRONIC STRUCTURE OF THE FLUORINATED DOUBLE â- WALL CARBON NANOTUBES PRODUCED USING DIFFERENT FLUORINATION METHODS

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Double-wall carbon nanotubes (DWNTs) have been synthesized by chemical vapor deposition method. Fluorination of DWNTs was performed using three different techniques: F2 treatment at high temperature, CF4 plasma treatment, and by gaseous BrF3 at room temperature. Raman spectra indicated that the inner shells remained intact in all fluorinated DWNTs. Fluorine content of the samples was determined from x-ray photoelectron spectroscopy. Comparison of the x-ray absorption near C K-edge spectra (XANES) of the fluorinated DWNTs showed the nanotubes are different in the density of unoccupied electronic states. The F

K-edge XANES spectra of the fluorinated DWNTs showed dependence of fluorine atoms positions on nanotube surface on fluorination conditions. Annealing of the fluorinated DWNT led to removing of the fluorination atoms from and this process depends on C-F bond strength.

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Metal-induced doping and edge effects in graphene devices probed by scanning photocurrent microscopy

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Graphene has been a topic of intense research in recent years both from fundamental and technological perspectives. Its linear energy dispersion around the Fermi level leads graphene quasiparticles to mimic relativistic Dirac fermions, as demonstrated experimentally both by electrical and optical studies. Furthermore, quasiparticles in graphene possess extremely high carrier mobilities, rendering graphene devices attractive for future applications in electronics. Toward this end, it is essential to first understand the operating mechanisms of such devices, which involve many aspects that have still not been explored. In this work, we evaluate by scanning photocurrent microscopy (SPCM) the effects of the electrical contacts and the flake edges on graphene devices. The observed photocurrent responses revealed the presence of electrostatic potential steps at the metal-graphene interfaces that act as transport barriers at the metal contacts. Moreover, it is demonstrated that the devices do not switch in a homogeneous way as they are brought from the p- to the n-type regime by electrostatic gating. Instead, a transversal p-n-p profile is observed around the Dirac point.

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Conductivity of CNT filled polymer melts under sinusoidal shear

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The application of carbon nanotubes (CNT) for tailoring polymer composites has drawn great attention over the last few years. Due to their large aspect ratio and specific surface, they are promising filler materials for mechanical reinforcement of polymers and, because of their outstanding electrical conductivity, also for the enhancement of the electrical conductivity of those materials. However, the electrical properties of such composites are very sensitive to the shear history the material has undergone during processing. In order to understand the influence of shear deformations on the conductivity on CNT filled polymer melts, we built up a rheometer setup with rheometer plates acting as electrodes, concurrently. By advanced electronic control of the rheometer we are able to overlay a constant shear and a sinusoidal shear rate. Both the resulting torque and the electrical conductivity can be measured perfectly synchronous with high acquisition rate. We will present the conductivity behaviour of multiwall CNT filled polymer melts under sinusoidal shear deformations of different strain amplitudes.

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Temperature modification of oxidized multiwall carbon nanotubes (ox-MWCNTs) studied by the electron spectroscopy methods

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Carbon nanotubes (CNTs) can be applied as promissing catalyst support due to excellent electrical conductivity, high surface area and good access of reactants to metallic catalyst deposited on CNTs. In the present work the temperature modification of ox-MWCNTs in the range from RT to 150 C was investigated. Their surface was studied by electron spectroscopy methods, i.e. XPS, XAES, EPES and EELS. The TEM showed irregular structures of bundled and non-uniform diameter ox-MWCNTs. Thermal desorption showed varying contributions of H2, H2O, CO and CO2 depending on the temperature. The H2O could diffuse from CNTs channels. The CO2 could originate from COOH groups, whereas the CO from OH and C=O groups. The content of oxygen at the ox-MWCNT surface decreased from 12.4 at. % to 9.8 at. %. The C 1s spectra showed increasing number of C sp2 bonds confirmed by the width of C KLL transitions (from 63 % to 74 %). The O 1s spectra indicated increasing content of aromatic C=O groups accompanied by decreasing content of aliphatic C=O, aliphatic and aromatic CâOH and COOH groups. Structural changes were observed in EELS spectra from increase and shift of the pi-plasmon.

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Combined STM/STS, TEM/EELS investigation of CNx-SWNTs

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We have studied the impact of nitrogen atoms on the electronic structure of C-

SWNTs by combining STM/STS and TEM/EELS.To this aim, CNx-SWNTs have been synthesized by vaporizing with a continuous laser a C:Ni/Y target under a nitrogen atmosphere. EELS analysis indicates a nitrogen concentration lower than 1 at.per cent and the existence of two different local environments of N atoms, the first one being a graphitic configuration where an N atom is simply substituted to a C atom, and the second one a more complex configuration such as the pyridinic like configuration. Using STM and STS, specific defects have been assigned to the presence of N atoms as they are not observed in pure C-SWNTs. They give rise, in images, to protusions extended over 3-5 nm and having a large periodicity. They also provoke a change in the helicity of the tube. At the apex of the defect, STS reveals the presence of two localized states within the band gap, one donor and one acceptor, shifted by about 0.3 eV from the Fermi level.These signatures indicate a complex defect, which could correspond to the second kind of environment identified in EELS.

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Thermal decomposition of C60H18

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Fullerene C60 is known to react with hydrogen gas with formation of various hydrofullerenes. However, reverse reaction of highly hydrogenated fullerene, which occurs at temperatures over 800K, results not only in recovery of pristine C60 but also in partial collapse of fullerene molecules. Starting material, C60H18, was produced by direct reaction of solid C60 with hydrogen gas at elevated conditions. Dehydrogenation products obtained in a broad range of temperatures and using various periods of heat treatment were characterized by XRD, IR spectroscopy, Raman spectroscopy and mass spectrometry. Hydrofullerene C60H18 exhibits fcc structure with increased cell parameter a=1.455 nm compared to pristine C60 (1.417 nm). Breakup of C-H bonds was observed for temperatures of heat treatment above 620K using IR and Raman spectroscopy. However, the cell parameter of fcc structure remained the same as for pristine C60H18 and even become higher when temperature of heat treatment was increased. Seemingly paradoxical increase of cell parameter correlates with partial collapse of fullerene molecules and formation of nanocarbon phase. It is proposed to use thermal decomposition of hydrofullerenes for synthesis of graphene-related materials and graphite nanoparticles.

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Resonance Raman Study of Phosphorous Doped Single-Wall Carbon Nanotubes

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Doping single-wall and multi-wall carbon nanotubes changes their physical and chemical properties. The most studied substitutional doped nanotubes are the ones containing boron and nitrogen, the nearest neighbors of carbon in the periodic table that can provide holes and electrons to the tube, respectivelly. Phosphorous is another electron donor to nanotubes, but fundamentally different from nitrogen because it belongs to a different row in the periodic table. In this work, substitutional phosphorous doping in single-wall carbon nanotubes is investigated by resonance Raman spectroscopy. We study the doping-induced changes in the radial brething mode (RBM), disorder-induced mode (D mand), graphitic G and G$'$ bands, drawing a comparative study with observations in boron and nitrogen doped tubes. Changes in the diameter distribution, resonance Raman cross-section, thermal transport, electron and phonon structure will be discussed.

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Determination of the tight-binding parameters of bilayer graphene by resonance Raman scattering

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In this work, the electronic and vibrational structure of bilayer graphene are investigated from a resonant Raman study of the 2D band using different laser excitation energies in the visible and near infrared range. The values of the tight-binding parameters of the Slonczewski-Weiss-McClure (SWM) model for bilayer graphene are obtained from the analysis of the dispersive behavior of the Raman features and compared with recent results from infrared measurements. Our results evidence a significant asymmetry between the valence and conduction bands of bilayer gra-

phene. The splitting of the two iTO phonon branches in bilayer graphene is also obtained from the experimental data and we show that the phonon renormalization is stronger for the totally symmetric phonon branch.

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Versatile growth of carbon nanotubes at low temperature by the equimolar C_2H_2-CO_2 reaction

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Chemical vapor deposition is considered to be the most viable process for in situ production of nanotubes integrated into a device. Regardless of the carbon source, synthesis is nowadays limited to classical decomposition reactions, for example, $C_xH_y \rightarrow$ xC + y/2H_2 and 2CO → C + CO_2.

Herein, we will report a newly discovered equimolar reaction between acetylene and CO_2 to produce CNTs. The overall reaction can be described by the following equations: $C_2H_2 + CO_2 \rightarrow 2C + H_2O + CO$ or $C_2H_2 + CO_2 \rightarrow C + 2CO + H_2$. An extensive characterization of the chemical mechanism will be presented. Without demanding pre-activation process of the catalyst , the equimolar C_2H_2-CO_2 reaction allows CNTs growth at temperatures well below 500 ◦C, on numerous functional materials like oxides, nitrides, carbides, borides or metals. As well, macroscopic objects built from aligned CNTs can be produced. It is an attractive synthesis pathway for the direct integration of CNTs into devices which do not support a high temperature processing of synthesis CNTs.

[1] A.Magrez, J.W. Seo, et al, Angew. Chem. Int. Ed. 46 (2007) 4.

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Experimental realization of metastable ferromagnetic phases in dilutely hydrogenated fullerenes

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We are presenting the recipes and cooking tips for preparing films of dilutely hydrogenated fullerenes H:C_{60}. Lowering the symmetry to the C_h group in the case of $C_{60}H$ and to C_v for $C_{60}H_2$ makes all the symmetric vibrations Raman active, and the number of modes appears in the spectra. DFT calculations of the Raman spectra at the B3LYP/3-21G level are compared with the experimental data. Under the laser treatment these exotic films form a rich variety of dimeric and polymeric structures, quite in contrast to usual hydrogenated fullerenes which do not polymerize at all, and to pristine CC_{60} which forms dimers and polymers bonded by two interfullerene Ï-bonds through the [2 + 2] addition. Dilutely hydrogenated fullerenes polymerize differently, forming both double bonded structures and single bonded ones. We have shown that double bonded polymerization of C_{60} :H leads to a metastable ferromagnetism which disappears due to the structural relaxation and formation of diamagnetic single bonded dimers.

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Molecule Nanotube Hybrids

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Single functional molecules are the basic elements of molecular electronics. A reliable contact between molecules and metal electrodes is still a challenge for fabricating single-molecule devices. Metallic single-walled carbon nanotubes (mSWCNT) have promising properties for their application as metallic electrode due to their low dimensionality, ballistic transport behaviour and stability against electromigration [1].

Our approach to produce mSWCNT-molecule-mSWCNT devices is as follows: First we assemble a low-resistance single mSWCNT device by dielectrophoretic assembling and subsequent conditioning [2]. Then we produce a gap of several nanometers size in the mSWNT by electrical breakdown, finally we implant custom tailored molecules. Our molecules possess a fluorescent part that shows luminescence at a specific wavelength. During electronic transport measurements on our molecule-nanotube hybrids we simultaneously measure the emitted light which gives us a molecule specific fingerprint.

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[2] C.W. Marquardt, Nano Lett. 9 (2008) 2767.

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^{13}C NMR investigation of cubane-fullerene $C_8H_8{\cdot}C_{60}$ cocrystals

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The rotor-stator molecular cocrystal $C_8H_8{\cdot}C_{60}$ (cubane–fullerene) has been investigated by ^{13}C nuclear magnetic resonance (NMR). The room-temperature spectrum obtained using ^{1}H–^{13}C cross-polarization technique exhibits two lines with chemical shifts identical with the shifts of the original molecular constituents demonstrating the lack of strong electronic interaction between C_{60} and C_8H_8.
The temperature dependence of the spin-lattice relaxation time of the fullerene component confirms the existence of a first-order orientational ordering transition around 145 K; above the transition temperature there is only one relaxation time whereas in the transition region two relaxation times with varying spectral weights can be observed. The spectrum remains narrow down to 90 K indicating that similarly to pristine C_{60}, the molecular reorientational motion is still fast in the ordered phase on the NMR time scale.

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Vibrational properties of graphene nanoribbons by first-principles calculations

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We investigated the vibrational properties of graphene nanoribbons by means of first-principles calculations on the basis of density functional theory. We find that the phonon modes of graphene nanoribbons with armchair and zigzag type edges can be interpreted as fundamental oscillations and their overtones. These show a characteristic dependence on the nanoribbon width. Furthermore, we demonstrate that a mapping of the calculated Γ-point phonon frequencies of nanoribbons onto the phonon dispersion of graphene corresponds to an “unfolding” of nanoribbons’ Brillouin zone onto that of graphene. We consider the influence of spin states with respect to the phonon spectra of zigzag nanoribbons and provide comparisons of our results with past studies.

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Relaxation and decoherence of spins in ^{15}N and ^{31}P in C$_{60}$

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The spin states of ^{15}N and ^{31}P atoms encapsulated in C$_{60}$ are quite interesting *per se*, as well as in the context of quantum information processing. Their application as quantum bits (qubits) has already been extensively investigated in the literature. In this contribution we present new results concerning the relaxation and decoherence phenomena observed in these systems. We address in particular the creation of entangled states in selective sublevel systems and their decoherence. Moreover we present methods for lengthening the intrinsic coherence time using specific multiple pulse electron spin echoes, which are also applicable to other spin qubits. Several scenarios will be compared.

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Lattice dynamic of h-BN: from a 2D-layer to a 3D solid

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We present a theoretical study of the lattice dynamics of hexagonal boron nitride (h-BN), considering the evolution of the phonon spectrum from a single layer to a multilayer- and 3D-solid. Particular emphasis is put on the interplay between valence and Coulomb forces between ions. Intra-plane valence forces are taken from a fifth-neighbor force-constant model derived from full in-plane phonon dispersions of graphite [Mohr et al. Phys. Rev. B 76, 035439 (2007)]. Inter-plane interactions are described partially by van de Waals forces. Coulomb interactions for intra-plane and inter-plane potentials are treated by the Ewald method. The phonon dispersion relations are derived throughout the Brillouin zones. The theoretical results are compared with experiments on elastic constants and optical phonons. Piezoelectric effects are discussed.

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Symmetry based analysis of the electron-phonon interaction in graphene

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Symmetry based analysis of the electron-phonon interaction in graphene is performed. Extraordinary physical properties are shown to be consequence of symmetry. The results are confirmed within full and TB DFT calculations and FC model.

Graphene has a diperiodic symmetry group DG80=$\mathbf{TD}_{6h}$. It is a single orbit system generated by DG3=$\mathbf{TC}_2$, with the stabilizer group isomorphic to $\mathbf{D}_{3h}$. Despite the large stabilizer this is a symmetry fixing set. Hence, its dynamical representation shows low diversity of the phonon modes symmetry.

It is these two facts which provide the extraordinary effect: There are non symmetric modes which are not vibronically coupled and thus might be responsible for stability of the honeycomb lattice. Symmetry also predicts vanishing of the electron-phonon interaction for quite a number of the normal displacements. Thus, lattice dynamics along these degrees of freedom is governed by the ion repulsion which leads to the anharmonic terms, being linear in absolute elongation. In particular, this effect is attributed to the K and Γ points of the BZ, giving insight into origin of the Kohn anomaly.

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Preparation and characterisation of SU8-carbon nanotubes composites

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SU8 is a highly chemical resistant near UV photoresist. This negative epoxy polymer is inexpensive and can be easily processed in high aspect ratio structures with standard photolithography. Therefore, it has a very broad range of applications, especially in the domain of micro and nanotechnologies (nanofluidic, nanoelectromechanical systems ...). However, SU8 is an insulating and brittle polymer. Therefore, we have prepared SU8/CNTs composite aiming at reinforcing the polymer and at enhancing its electrical and thermal properties.

At first, we have optimized the mixing conditions (process, solventâ) and studied the influence of the CNTs functionalisation in order to enhance the CNTs dispersion within the polymeric matrix as well as to improve the interaction between CNTs and SU8. So far, homogeneous SU8/CNTs composites have been obtained and layers with tunable transparency and thickness have been prepared. Results of the mechanical, electrical and thermal properties characterization of the composites will be presented.

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Resonance Raman scattering of metallic and semiconducting single-wall carbon nanotubes

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Resonance Raman spectroscopy is a powerful tool to study the phonon and the electronic states of single-wall carbon nanotubes (SWCNTs). In previous studies, however, the detailed analysis has been limited by the mixed Raman signals from the co-existing metallic and semiconducting SWCNTs in as-grown samples. Here, we present the results of the resonance Raman scattering performed on high purity metallic and semiconducting SWCNTs. The metallic and the semiconducting SWCNTs were prepared using a density gradient ultracentrifugation method. Interestingly, for the intermediate frequency modes (IFMs) between 600 and 1100 cm-1, sharp peaks with steplike dispersive resonance behavior were observed only for semiconducting SWCNTs. In addition, it was found that the metallic SWCNTs showed largely different frequency of the D-mode and some other high-energy modes from those of semiconducting SWCNTs. We will discuss possible physical backgrounds of the difference observed in Raman response between the metallic and the semiconducting SWCNTs.

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The radial breathing mode in CdSe nanorods

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We performed *ab initio* calculations of the vibrational properties of bare CdSe nanowires and CdSe/ZnS core/shell nanowires and found a radial breathing mode (RBM). We calculated the modes' frequency for various diameters and sets of bare CdSe nanowires and CdSe/ZnS core/shell nanowires to determine the diameter dependence of the modes' frequency. The frequency of this mode is strongly diameter dependent. We experimentally confirm the existence of the radial breathing mode CdSe nanorods by Raman spectroscopy and it can be used to estimate the nanorod diameter from a Raman measurement alone.

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Spectroscopy of Single-Walled Carbon Nanotubes in Aqueous Surfactant Dispersion

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Optical studies of single-walled carbon nanotubes (SWNTs) have advanced greatly since the discovery of structured near-infrared band gap photoluminescence from nanotubes dispersed in aqueous surfactant suspensions [O'Connell, Science, 2002, 297, 593]. In our work, we have solubilised different batches of SWNTs in Milli-Q water using SDBS. SWNT samples have been chosen by varying three different parameters: the percentage of impurities present in the tubes, the amount of defects introduced in their graphitic structure and/or the functional groups expressed on their surface. Near-infrared Absorption and Emission Spectroscopy as well as Raman Spectroscopy have been carried out on all solutions. The differences in the spectroscopic results have been evaluated in relationship with the purity, oxidation and functionalization grade of the SWNTs utilized. Moreover, the resulting spectral data have been analyzed, using established findings in SWNT optical spectroscopy, to provide a detailed description of the semiconducting SWNT content of the samples: diameter distribution and (n,m)-species relative abundance have been assigned from fluorimetric intensities.

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Raman spectroscopy of single wall carbon nanotubes functionalized with terpyridine-ruthenium complexes

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A resonant Raman scattering study on single-wall carbon nanotubes (SWCNTs) decorated with terpyridine-Ru(II)-terpyridine (tpy-Ru(II)-tpy) moieties is presented. We compare samples efficiently synthesized bearing either monomeric or polymeric side chain tpy-Ru(II)-tpy dicomplexes following the âgrafting toâ and âgrafting fromâ approaches, respectively [1]. From the extracted resonance profiles of the radial breathing modes (RBMs) the chiral indices of the corresponding tubes are assigned [2]. We observe significant changes in the transition energies and the widths of the resonance windows due to chemical modification of SWCNTs. Interestingly, the polymer-wrapped sample exhibits significant RBM frequency shifts accompanied with drastic intensity alterations [3]. We discuss our findings in the context of a possible selectivity to certain tube species or diameters.

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Sequence-Specifically Addressable DNA-SWCNT Complexes

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Single-walled carbon nanotubes (SWCNT) are attractive building blocks for molecular electronics and novel materials. Generating functional architectures with SWCNTs requires methodologies for dispersing the nanotubes, purifying them, and depositing them within a functional molecular context. We have previously reported the effect of length and sequence of DNA on complexes with carbon nanotubes. We showed that DNA-SWCNT complexes are kinetically too stable to allow for hybridization to extraneously added, complementary DNA strands. This prompted us to develop new DNA sequence motifs that allow for hybridization to complementary strands and solubilization of SWCNTs simultaneously. Here we report that hairpin-forming oligodeoxynucleotides give suspension of SWCNTs that are more concentrated than those reported for other DNA sequences. Further, the resulting complexes bind single-stranded DNA sequence-specifically, as demonstrated for fluorophore-labeled targets. Finally, we show that the designed non-covalent complexes can be formed with SWCNTs that are predominantly of a single helicity, purified via density gradient ultracentrifugation.

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Sensing near to mid infrared light with a fullerene/silicon hybrid heterojunction

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We demonstrate a low energy infrared light sensing scheme based on a fullerene-derivative (PCBM)/boron doped silicon hybrid heterojunction. On top of the p-Si substrate a PCBM thin film has been prepared by spin-coating. By thermal evaporation of aluminum, ohmic contacts to PCBM as well as to p-Si are maintained. In dark, an almost ideal Schottky diode behaviour is observed. Under IR illumination,the heterojunction PCBM/Si absorbs in a lower energy range than the energy gaps of the semiconductors, and generates a primary photoâcurrent. The IV-characteristics under broadband IR light illumination at 80K features an open circuit voltage of 0.5V and a short-circuit current in the range of several nA/cm2. The photo-current between 80K and 220K has been spectrally resolved by Fourier Transform IR spectroscopy. Above a threshold of 0.4 eV, the photo-current increases linearly up to the fundamental energy gap of silicon (1.17 eV). A theoretical model describing the absorption process across the heterojunction will be presented. The scientific relevance and the simple CMOS compatible fabrication process make the presented hybrid approach a promising candidate for widespread applications.

49
Purity Evaluation of Single-Wall Carbon nanotubes based on Raman Spectroscopy

Daisuke Nishide[1] Yasumitsu Miyata[1] Kazuhiro Yanagi[1] Takeshi Tanaka[1] Hiromichi Kataura[1]
[1]Nanotechnology Research Institute (NRI), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba

Purity evaluation is an important problem awaiting solution in the fundamental research field and the consumer market of single wall carbon nanotube (SWCNT). For the quantitative purity evaluation, we need probe signals which are proportional to the abundance of SWCNTs in the sample and a 100% purity SWCNT sample as a standard. Intrinsic optical absorption intensity of SWCNTs can be used as a probe signal for the purity evaluation. However, a baseline correction is required to obtain the accurate intensity of SWCNTs from the spectrum because a tail of the broad UV absorption is overlapping. On the other hand, Raman intensity is also related to the intrinsic optical absorption of SWCNT by way of the resonance effect. In this paper, we show that the Raman signal from the isolated SWCNTs in a water solution is proportional to the abundance of SWCNTs. Further, extremely purified SWCNT sample can be obtained easily by an ultracentrifugation as the 100% standard. Finally we propose a new method for quantitative purity evaluation of SWCNTs based on Raman spectroscopy. We will introduce the detailed protocol and will demonstrate the purity of various SWCNTs evaluated by this method.

50

Effect of ammonia on the growth behavior of nitrogen-doped carbon nanotubes.

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Nitrogen-doped carbon nanotubes are grown on e-beam deposited thin metal films (cobalt/iron) by chemical vapour deposition. The approach uses ammonia as supporting gas to form nano catalyst particles in the pretreatment phase. Ammonia is also used as the nitrogen source. The effect of ammonia on the grown structures at different temperatures (800 °C and 900 °C) is investigated by SEM, TEM and Raman spectroscopy. It could be shown that by the support of ammonia carpets of aligned CNTs can be grown even on thicker metal films (5nm) than usually used. At the same time ammonia is inducing a high amount of defects but this effect changes significantly with temperature. At 800 °C defects are clearly ammonia induced. At 900 °C this mechanism reduces or even inverts.

51

Carbon Nanotube Containing Medium as a Saturable Absorber for Diode-Pumped YAG:Nd Solid State Laser Operated at Wavelength 1.32 μm

Petr A. Obraztsov[1] Sergey V. Garnov[2] Elena D. Obraztsova[2] Anatoly S. Lobach[3] Anatoly A. Sirotkin[2] Yury P. Svirko[1]
[1]Department of Physics and Mathematics, University of Joensuu, Joensuu
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A diode pumped passively mode-locked YAG:Nd laser operated at wavelength 1.32 μm has been developed using a novel saturable absorber based on single-wall carbon nanotubes incorporated in a polymer matrix. Laser pulses with the output energy up to 70 μJ and the duration of 50 ps have been generated. A stable mode-locking regime has been obtained with the pump frequency up to 1kHz. The single-wall carbon nanotubes synthesized by a high pressure CO decomposition (HiPCO) technique have been used due to the appropriate working spectral range [1]. The individual nanotubes were distributed into a polymer (carboxymetylcellulose) matrix. An absorption spectrum and kinetics of electron excitation relaxation have been measured by a pump-probe technique. [1]. S.V. Garnov, S.A. Solokhin, E.D. Obraztsova, A.S. Lobach, P.A. Obraztsov et al. âPassive mode-locking with carbon nanotube saturable absorber in Nd:GdVO4 and Nd:Y0.9Gd0.1VO4 lasers operating at 1.34Î¼mâ, Laser Physics Letters 4 (2007) 648. The work was supported by RFBR projects 08-02-91755-AF and 07-02-91033AF.

52

GRAPHENE LAYERS ON THE SURFACE OF GRAPHITE FLUORIDE C2F: SYNTHESIS, STRUCTURE, AND ELECTRICAL CONDUCTIVITY

Alexander V. Okotrub[1] Lyubov G. Bulusheva[1] Konstantin S. Babin[1] Igor P. Asanov[1] Artem V. Guselnikov[1] Nikolay F. Yudanov[1]
[1]Nikolaev Institute of Inorganic Chemistry SB RAS, Siberian Branch Russian Academy of Science, Novosibirsk

Fluorination of graphite using a gaseous BrF3 at room temperature yields graphite fluoride of a C2F composition. The material consists of light transparent plates, which are resistant to the electrical current. We developed procedure for reduction of the upper layers of the graphite fluoride and obtained thin current-conductive graphite layers on the surface of insulating C2F matrix. The surface of pristine graphite fluoride has mosaic structure from the fluorinated regions having a size of 2 nm. Due to weak bonding of fluorine atoms with the surface carbon atoms the upper layers of C2F are easy restored to the graphitic state under the action of water vapors. The measurement of relative intensity of angle-resolved X-ray photoelectron C 1s spectrum excited by various wave-length radiations has estimated that the thickness of graphitic layers is less than 1 nm. A change in the structure of graphite fluoride under the reducer action was studied by atomic-force microscopy. An electrical conductivity of the samples was measured depending on the restoring degree.

53

Synthesis-kinetics of vertically aligned carbon nanotubes

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[3]School of Chemistry, Edinburgh University, Scotland

Before the properties of carbon nanotubes can be fully exploited in the many proposed applications their synthesis has to be understood and controlled.

Vertically aligned nanotube arrays with heights over 800 μm have been grown using acetylene with iron as catalyst on alumina support in TCVD. The nanotubes were multi-walled and the number of walls increased with increasing partial pressure of acetylene.

The kinetics was studied to link the macroscopic properties to the microscopic processes of synthesis. It was found that the addition-rate of carbon was proportional to the coverage of acetylene molecules on the catalyst nanoparticle. The poisoning of the catalyst was suggested to be partly due to gas-phase pyrolysis.

In certain conditions of synthesis it has been found that the macroscopic pattern of the catalyst areas influenced the microscopic properties of the CNTs. Larger areas of catalyst gave longer carbon nanotubes, but with a similar amount of carbon atoms since they had fewer number of walls. To explain the observations a model based on acetylene depletion was proposed. The results indicate that the number of walls was determined at an early stage of the synthesis.

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Concept of Graphene as a Macromolecule: Spectrum, Conductance, and Tunneling

Alexander I Onipko[1] Lyuba Malysheva[1]
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The exact model description of pi electrons in graphene as an alternant plane macromolecule is elaborated. The model suggests an instructive alternative to the approach with reference to the honeycomb lattice periodic in the A and B sublattices. New results on the spectrum, conductance, and tunneling will be reported.

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Transparent Conductive Film Using Oligo-Graphite

Hye Jin Park[1] Viera Skakalova[1] Siegmar Roth[2]
[1]Max Planck Institute for Solid State Research, Stuttgart
[2]SINEUROP Nanotech GmbH

The transparent conductive electrode using single walled carbon nanotubes (SWNTs) has been studied intensively for last decade. Recently, graphite nanoplatelets (GNPs) have emerged as a promising filler which shows enhanced thermal and electrical conductivity in composite materials. In this study, we present the electrical conductivity as well as transmittance of the thin films which could be prepared by transferring oligo-graphite, which has less than 10 layers of graphenes, onto polycarbonate film. Oligo-graphite was synthesized on Ni coated SiO2/Si substrate via CVD method using CH4 and H2 gases at 1000 oC. The synthesized oligo-graphite was transfered to polycarbonate (PC) film via etching of nickel layer by hydrochloric acid and washed with distilled water. The film transmittance and sheet resistance could be controlled by changing the synthetic condition of the oligo-graphite as well as by doping the thin film. The films were characterized by Raman, optical microscopy, SEM, and UV/Vis/NIR spectroscopy.

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Characterization of dye molecules and carbon nanostructures by tip-enhanced Raman spectroscopy

Niculina Peica[1,2] Serge Röhrig[3] Andreas Rüdiger[3,4] Katharina Brose[1] Christian Thomsen[1] Janina Maultzsch[1]
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[3]Institute of Solid State Research and Center of Nanoelectronic Systems for Information Technology, Research Center JÃ¼lich, Leo-Brandt-St., 52425 Jülich, Germany
[4]INRS Énergie, Matériaux et Télécommunications, 1650 boul. Lionel Boulet, J3X 1S2 Varennes (Québec), Canada

The recent development of Raman instrumentation with submicron spatial resolution has created new possibilities to investigate nanomaterials such as carbon nanotubes and nanofibers or other nanosized particles. Recently, a new approach for nanosized lateral resolution in Raman spectroscopy, called tip-enhanced Raman spectroscopy (TERS), sometimes referred to as „apertureless scanning near-field optical microscopy (SNOM)“has been developed [1]. TERS is a high-sensitivity and high spatial-resolution analytical technique based on the strong field enhancement provided by a sharp metallic tip. Near-field Raman scattering has been successfully used to study the interaction between a metal-coated tip and carbon nanostructures [2,3]. The enhanced and localized surface plasmons in the apex provide high resolution imaging as well as the detection of vibrational modes that are not well visible with confocal Raman spectroscopy. We present confocal Raman and TERS spectra of dye molecules and other nanostructures. [1]. R.M. Stöckle et al. Chem. Phys. Lett. 318 (2000) 131. [2]. Y. Inouye et al. Proc. SPIE 6324 (2006) 63240K. [3]. A. Hartschuh et al. Surf. Interface Anal. 38 (2006) 1472.

57

Raman Characterization of the Antipodal C_{60} and Anthracene Bis-Adduct

Rudolf Pfeiffer[1] Hans Kuzmany[1] Bernhard Kräutler[2] Christian Kramberger[1] Manuel Melle-Franco[3]
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[2]Institute of Organic Chemistry, University of Innsbruck, Austria
[3]Physical Sciences, University of Kent, UK

In order to produce 1D spin chains by filling magneto-fullerenes into SWCNTs we stumbled upon the problem of reliably adjusting the fullerene spacing. Simulations suggest that the antipodal bis-adduct of C_{60} and anthracene is a good candidate for the engineering of the fullerene spacing.

First, the mono-adduct was produced which was then turned into various bis-adducts by a Diels-Alder reaction. In a final purification step the almost pure antipodal bis-adduct was obtained. The FT-Raman spectra of the adducts showed strong C_{60} derived peaks. Additionally, they exhibited a number of smaller peaks due to the reduced symmetry. No obvious anthracene peaks could be found. The main proof of the functionalization was the increased number of peaks in the adduct spectra and a downshift of the $A_{\mathrm{g}}(2)$-derived modes by 5 and 10 cm^{-1} for the mono- and bis-adducts, respectively. Additionally, the adducts exhibited strong peaks at the unshifted $A_{\mathrm{g}}(2)$ position. This was taken as a hint for a decay of the adducts until calculated Raman spectra using Gaussian also showed these peaks.

This work was supported by FWF-project I83-N20 (ESF IMPrESS).

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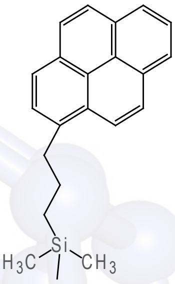

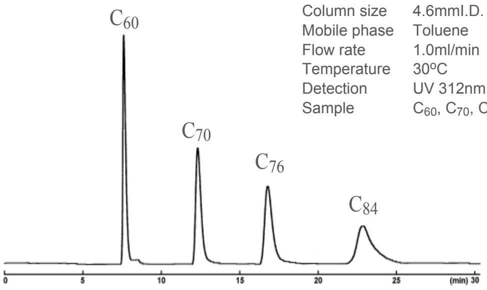

Column size	4.6mmI.D. x 250mm
Mobile phase	Toluene
Flow rate	1.0ml/min
Temperature	30°C
Detection	UV 312nm
Sample	C_{60}, C_{70}, C_{76}, C_{84}

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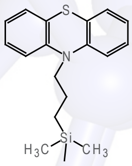

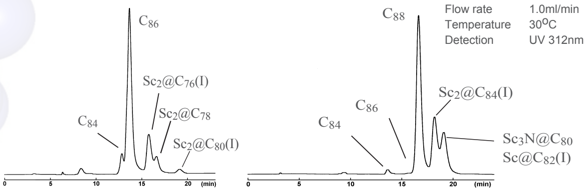

Column size	4.6mmI.D. x 150mm
Mobile phase	Toluene
Flow rate	1.0ml/min
Temperature	30°C
Detection	UV 312nm

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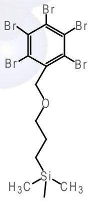

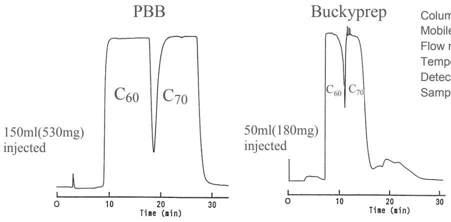

Column size	20mmI.D. x 250mm
Mobile phase	Toluene
Flow rate	18ml/min
Temperature	Room temperature
Detection	UV 285nm
Sample	Crude fullerenes (3.5mg/ml)

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Optics of carbon nanotubes

8:30 – 9:30	V. Perebeinos, US *Understanding environmental effects on the electronic and vibrational excitations and dynamics in carbon Nanotubes*
9:30 – 10:00	R. Saito, JP *Exciton states and phonon softening phenomena in single wall carbon nanotubes*
10:00 – 10:30	Coffee break
10:30 – 11:00	A. Hartschuh, DE *Near-field optical investigations of individual single-walled carbon nanotubes*
11:00 – 11:30	H. Telg, DE *Characterization of isolated metallic and semiconducting nanotubes by Raman spectroscopy*
11:30 – 12:00	A. Jorio, BR *Disorder in* sp^2 *nano-carbons: doping, ion bombardment and substrate interaction*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	S. Maruyama, JP *Spectral features due to dark exciton in photoluminescence map of single-walled carbon nanotubes*
19:00 – 19:30	Malic, DE *Linear optical spectra and relaxation dynamics in single-walled carbon nanotubes*
19:30 – 20:00	B. Lounis, FR *Optical spectroscopy of individual single-walled cCarbon nanotubes*
20:00 – 20:30	Z. K. Tang, HK *Resonant Raman of 0.3 nm single-walled carbon nanotubes*

Wednesday, March 11

8:30

Understanding environmental effects on the electronic and vibrational excitations and dynamics in carbon nanotubes

Vasili Perebeinos
Watson Research Center, IBM - Watson, Yorktown Heights

The electronic, vibrational, and excited states dynamics in carbon nanotubes (CNT) can be strongly influenced by the environmental effects. In this talk we will review recent advances in the role of the CNT environment on the electronic states, phonon and exciton dynamics probed by the optical spectroscopy.
The transport properties of CNTs on polar substrates are determined by the surface polar phonon (SPP) mode scattering and can be modified by the choice of the insulating substrate. SPP scattering determines the low field mobility in CNTs on SiO_2 even at room temperatures and it serves as an efficient channel for heat dissipation in CNTs under high bias conditions. The latter can be probed by the Raman spectroscopy to map out the electrically-excited phonon populations and the power dissipation pathways in functioning carbon nanotube transistors.
Finally, we address the long puzzling question regarding the nature of the dominant decay channel of the low energy excited states and the potential of optoelectronic applications of CNTs. The non-radiative lifetime of strongly bound excitons is predicted to depend strongly on the free carrier density.

9:30

Exciton states and phonon softening phenomena in single wall carbon nanotubes

Riichiro Saito[1] Kenichi Sasaki[2] Jin Sung Park[1] Kentaro Sato[1]
[1]Department of Physics, Tohoku University, Sendai
[2]Advanced Sciences of Matter, Hiroshima University

Two subjects on optical properties of single wall carbon nanotubes(SWNTs) are discussed. The first subject is a photoluminescense (PL) problem of SWNTs. Because of the symmetry of a SWNT, the lowest exciton states is an optically forbidden state (dark exciton state). We will present our numerical calculation of the exciton and show some problems in comparison with the recent PL measurements under the magnetic field. Another subject is phonon softening phenomena in metallic carbon naotubes, which are known as the Kohn anomaly of phonons. Because of anisotropic electron-phonon interaction in the k space around the K point, resonance Raman spectra of an isolated SWNT shows anomalous phonon softening phenomena which depend on chiral angle. We will explain the chirality dependent phonon softening phenomena by a time reversal gauge field.

10:30

Near-field optical investigations of individual single-walled carbon nanotubes

Achim Hartschuh[1] Huihong Qian[1] Carsten Georgi[1] Miriam Boehmler[1] Tobias Gokus[1] Lukas Novotny[2] Paulo Araujo[3] Ado Jorio[3] Mark C. Hersam[4]
[1]Department Chemie und Biochemie and CeNS, LMU Muenchen, Germany
[2]The Institute of Optics, University of Rochester, Rochester, NY, USA
[3]Departamento de Fisica, UFMG, Belo Horizonte, Brazil
[4]Department of Materials Science and Engineering and Department of Chemistry, Northwestern University, Evanston, Illinois, USA

We investigated single-walled carbon nanotubes on substrates using tip-enhanced near-field optical microscopy (TENOM) [1]. TENOM exploits the enhanced electric fields in close proximity to a sharp metal tip to locally increase both excitation and emission rates resulting in excellent spatial resolution ($<$15 nm), and high detection sensitivity. Simultaneous detection of tip-enhanced Raman scattering and photoluminescence (PL) allowed us to explore the correlation between strongly localized PL and charged doping sites [2]. DNA-wrapping of nanotubes was found to result in pronounced emission energy variations on a 10 nm length scale [3]. Surprisingly, DNA-wrapped nanotubes remain highly luminescent on metal films indicating additional field enhancement through the interference of metal-induced near-field modes. Coupling to these modes also leads to increased Raman scattering and substantial lifetime shortening of the emissive exciton state to below 3 ps. Finally, we report on our efforts to combine time-resolved PL techniques and TENOM. [1] A. Hartschuh, Angew. Chem. 47, 8178 (2008). [2] I. O. Maciel et. al, Nature Mat. 7, 878 (2008). [3] H. Qian et. al, Nano Lett. 8, 2706 (2008).

11:00

Characterization of isolated metallic and semiconducting nanotubes by Raman spectroscopy

Hagen Telg[1] Martin Fouquet[2] Janina Maultzsch[1] Yang Wu[3] Bhupesh Chandra[4] James Hone[4] Tony F. Heinz[3] Christian Thomsen[1]
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[2]Department of Engineering, University of Cambridge, Cambridge CB3 0FA, United Kingdom
[3]Departments of Electrical Engineering and Physics, Columbia University, New York 10027, USA
[4]Department of Mechanical Engineering, Columbia University, New York 10027, USA

Raman spectroscopy is a well established method to probe the presence of metallic nanotubes in a typical carbon nanotube sample, containing a large variety of different types of nanotubes. We show that experience based on nanotube ensembles

can not be transferred directly to experiments on isolated nanotubes. Resonance conditions and a precise analysis of the lineshapes of the Raman modes are necessary to discriminate metallic from semiconducting nanotubes. We analyze the high-energy Raman modes (HEMs), G^+ and G^-, in a pair of one metallic and one semiconducting nanotube grown across a 100 μm wide slit. By combining Rayleigh scattering with Raman resonance profiles of the radial breathing mode and the HEMs, we show that the two peaks, G^- and G^+, originate from different nanotubes. The G^- peak is the LO mode of the metallic tube; it is broadened and down shifted due to strong electron-phonon coupling. The G^+ peak is due to the LO mode in the semiconducting tube. We conclude that the presence of the G^+ peak at 1590 cm^{-1} in an assumed single isolated metallic nanotube very likely originates from an additional semiconducting nanotube.

11:30

Disorder in sp^2 nano-carbons: doping, ion bombardment and substrate interaction

Ado Jorio
Departamento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte

Disorder effects in sp^2 carbon systems are studied experimentally. In graphene and graphite, the effect of ion bombardment in the real and momentum spaces are correlated, as obtained by scanning tunneling microscopy and Raman spectroscopy measurements. In carbon nanotubes, charging effects due to substitutional doping (with boron, nitrogen and phosphorous) and tube-substrate interactions are studied using Raman spectroscopy, near-field spectroscopy and microscopy, atomic force microscopy and electric force microscopy. The observed phenomena are explainned based on the properties of electrons and phonons in the respective sp^2 carbon systems.

18:30

Spectral features due to dark exciton in photoluminescence map of single-walled carbon nanotubes

Shigeo Maruyama
Department of Mechanical Engineering, The University of Tokyo, Tokyo

Optical absorption by excitonic phonon sideband in photoluminescence (PL) excitation spectra [1] is well recognized as due to the strong phonon coupling to dark exciton with slightly higher energy than bright one. Here, we performed detailed PL spectroscopy studies of three different types of single-walled carbon nanotubes (SWNTs) by using samples that contain essentially only one chiral type of SWNT, (6,5), (7,5), or (10,5). The observed PL spectra unambiguously show the existence of an emission sideband at about 145 meV below the lowest singlet excitonic (E11) level. We find that the energy separation between the E11 level and the sideband is almost independent of the SWNT diameter. Based on this, we ascribe the origin

of the observed sideband to coupling between K-point TO phonons and dipole-forbidden dark excitons [2]. Furthermore, absorption features by cross-polarized excitations [3] and existence of quasi-dark absorption in cross-polarized excitation will be discussed.
[1] Y. Miyauchi, S. Maruyama, Phys. Rev. B, 74 (2006) 35415. [2] Y. Murakami, S. Maruyama, arxiv.org/abs/0811.4692. [3] Y. Miyauchi, M. Oba, S. Maruyama, Phys. Rev. B 74 (2006) 205440.

19:00
Linear optical spectra and relaxation dynamics in single-walled carbon nanotubes

Ermin Malic[1] Matthias Hirtschulz[1] Janina Maultzsch[2] Stephanie Reich[3] Andreas Knorr[1]
[1]Institut für Theoretische Physik, Technische Universität Berlin
[2]Institut für Festkörperphysik, Technische Universität Berlin
[3]Fachbereich Physik, Freie Universität Berlin

We show the potential of the density matrix theory for investigating optical properties of carbon nanotubes (CNTs). The theory is based on Bloch equations describing the dynamics of population and transition probabilities. In combination with TB wavefunctions, the approach allows microscopic calculation of linear and nonlinear optical properties of arbitrary CNTs. Its advantage lies in the straightforward inclusion of non-equilibrium many-particle effects, such as relaxation of electrons and phonons.
We illustrate the strength of the theory by performing calculations of excitonic absorption and Rayleigh scattering spectra for arbitrary CNTs: Kataura plots for excitation and binding energies are shown. Chirality dependence of the oscillator strength is investigated showing enhanced intensity for tubes with increasing chiral angle. We achieve good agreement with measured Rayleigh scattering spectra for metallic CNTs - with respect to peak splitting, intensity ratio, and peak asymmetry. The potential of our approach is further illustrated by investigating Coulomb driven intra-subband relaxation dynamics in CNTs. We find relaxation times on the fs timescale depending on the diameter.

19:30
Optical spectroscopy of individual single-walled carbon nanotubes

Brahim Lounis
CPMOH, CNRS and Bordeaux University, Talence

Current methods for producing single-walled carbon nanotubes (SWNTs) lead to heterogeneous samples containing mixtures of metallic and semiconducting species with a variety of lengths and defects. Optical detection at the single nanotube level offer the possibility to examine these heterogeneities provided that all SWNT types are equally well detected. Photothermal Heterodyne technique allows to perform highly sensitive imaging and absorption spectroscopy of individual small diameter SWNTs. Because it probes light absorption, the method enables identification of both semiconducting and metallic SWNTs. Using timeâresolved and cw luminescence spectroscopy, the absorption cross section of highly luminescent individual single-walled carbon nanotubes is determined. A mean value of 10-17 cm2 per carbon atom is obtained for (6,5) tubes excited at their second optical transition, and corroborated by single tube photothermal absorption measurements. Biexponential luminescence decays are systematically observed, with short and long lifetimes around 45ps and 250ps. This intrinsic behavior is attributed to the band edge exciton fine structure with a dark level lying a few meV below a bright one.

20:00

Resonant Raman of 0.3nm single-walled carbon nanotubes

Zi Kang Tang[1] J. P. Zhai[2] R. Saito[3] Ping Sheng[1]
[1]Hong Kong University of Science and Technology, Hong Kong
[2]College of Electronic science and Technology, Shenzhen University,
[3]Department of Physics, Tohoku University and CREST, JST,

Nano-porous single crystals can serve as ideal nano-reactors and assume variety of nano-structures those are usually not stable in free space. Their mono-dispersed porous with a macro-size of crystal, their optical transparency and electrical insulating properties, all make them attractive hosts for numerous applications. The periodic array of crystal porous makes it possible to build a quasi-3D structure for carbon nanotubes which is of importance for making optical and transport devices as it is. Using aluminophosphate porous single crystal of AlPO4-11 (AEL) as the template, we fabricated smallest single wall carbon nanotubes (SWNTs) with a diameter of only 0.3 nm. Energetically, the 0.3 nm SWNTs are not stable in free space, confinement in the nano-channels makes them very stable. Polarized and resonant Raman scattering revealed that these 0.3nm SWNTs are of (2,2) armchair symmetry. Interestingly, the (2,2) SWNT has two metastable ground state corresponding to two slightly different lattice constants in the axial direction, one state is metallic and the other is semiconducting.

Applications of carbon nanotubes

8:30 – 9:30	R. Baughman, US *Nanotube applications: from fascinating dreams to increasingly the marketplace*
9:30 – 10:00	D. Carroll, US *Progress toward negative index lenses*
10:00 – 10:30	Coffee break
10:30 – 11:00	C. Kramberger, AT *Sparse random arrays of pristine and doped carbon nanotubes: a tuneable meta material*
11:00 – 11:30	A. Bruinink, CH *In vitro effects of carbon based material*
11:30 – 12:00	Y. H. Lee, KR *Doping strategy of carbon nanotubes*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	R. C. Haddon, US *Advances in the chemistry and applications of carbon nanomaterials*
19:00 – 19:30	G. S. Duesberg, IE *Synthesis and characterisation of ultra-thin conducting carbon films*
19:30 – 20:00	J. O. Lee, KR *Sensing mechanism behind the metal-decorated SWNT-FETs*
20:00 – 21:00	Poster Session III – THU

Thursday, March 12

8:30

Nanotube applications: from fascinating dreams to increasingly the marketplace

Ray Baughman[1] Ali Aliev[1] Jiyoung Oh[1] Mikhail Kozlov[1] Alexander Kuznetsov[1] Shaoli Fang[1] Alexander DeFonseca[1] Raquel Robles[1] Marcio Lima[1] Mohammad Haque[1] Yuri Gartstein[1] Mei Zhang[2] Anvar Zakhidov[1]
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In a moment of foolishness, the speaker agreed to expand a talk on a fundamentally new type of carbon nanotube artificial muscle to one that provides an applications perspective for the entire nanotube area. This abstract describes only the first half of this talk. We have developed a fundamentally new type of artificial muscle, which operates in air to generate giant strokes and stroke rates of 220% and 3.7 x 104%/s, respectively. Charge-driven resonant and dc linear actuation result for volt to kilovolt drive voltages, and temperatures from below 80 K to above 1900 K. Using mechanical and electrical resonances, these artificial muscles provided ±30% oscillatory actuation at a kHz when driven by 10 Vrms. In the high modulus direction, where actuator stroke is a few percent, stress generation was 32-fold higher than for natural muscles. Actuation in this direction differs in sign from that in sheet width and thickness directions. We theoretically explain this sign reversal using giant observed Poissonâs ratios of up to 15, which provide a negative linear compressibility for the sheets.

9:30

Progress toward negative index lenses

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Developing Veselago's negative index materials for imaging applications in the visible regime has proven challenging due to the exponential loses in many materials experienced at short wavelengths. To be sure, there have been some demonstrations of negative refraction from systems in which hyperbolic dispersion exists (the permittivity is negative, but not the permeability), as well as some intriguing suggestions from nanolithographed split-ring resonator systems. However, to date a true demonstration of focusing and imaging in either the hyperbolic or resonant systems hasnât been forthcoming. In this work, we describe the use of self assembly methods to construct both hyperbolic and resonant lenses. The optical properties of assembled and aligned nanorod array â based „hyperbolic dispersion“lenses are described using diffractometry and interferometry. We then demonstrate imaging

through such a system which is consistent with our expectations for a negative index lens. From this structure we can now add resonant components to address the magnetic component of the index. Calculations indicate complete phase recovery will be achieved for such a lens at thicknesses of only a few microns. Preliminary optical data will be presented on these structures.

10:30
Sparse random arrays of pristine and doped carbon nanotubes: a tuneable meta material

Christian Kramberger[1] Ralf Hambach[2] Friedrich Roth[3] Roman Schuster[3] Roberto Kraus[3] Martin Knupfer[3] Erik Einarsson[4] Shigeo Maruyama[4] Lucia Reining[2] Thomas Pichler[1]
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Sparse arrays of aligned carbon nanotubes are a fairly dilute meta-material with strongly polarized dielectric properties. Angle resolved electron energy loss-spectroscopy evidences twofold plasmons for the π and the σ interband excitations in freestanding single wall carbon nanotubes. The bare existence of twofold plasmon dispersions is a novelty as compared to conventional bulk material, like graphite. These excitations are identified as a dispersive plasmon propagating along the nanotubes axis and its non-dispersive localized counterpart. The on-axis response is quantitatively identified as the in-plane response of a bare graphene sheet. Further, the dielectric properties of this system can be accurately tailored in *in situ* potassium intercalation. We evidence the emergence of a tuneable intraband charge career excitation. The dispersion of the new plasmon shows that it is the surface plasmon of a metallic meta material. These findings are indeed a critical empirical test for our understanding of strongly polarized nano-meshed meta-materials.

11:00
In vitro effects of carbon based materials

Arie Bruinink[1] Ursina Tobler[1] Sabrina Hasler[1] Pius Manser[1] Peter Wick[1]
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Carbon based materials are increasingly in the focus of interest because of their very specific mechanical and electrical characteristics. The increased knowledge about the applicability results in a steadily and rapid increase in number of patents. Concurrently, the production of, and as result of that the exposure to, these materials will increase in the near future. However numerous recent publications prove that carbonanotubes (CNT) may induce adverse effects after exposure. So far not much is known about their toxicomechanism. In the present study we determined single walled CNT (SWCNT) concentration-time â effect relationships.

We found that dependent on the parameter measured and purity of the material peak concentrations or exposure duration and by that the area under the curve (AUC) is the key factor defining the toxicity. In addition, it was investigated in how far assays like MTT-test and the reactive oxygen species (ROS) test based on 2',7'-dichlorofluorescin diacetate (H2DCF-DA) conversion are applicable for investigating SWCNT toxicity. At the SWCNT concentration range used of both assay only the H2DCF-DA test had clear-cut limitations in its use.

11:30
Doping strategy of carbon nanotubes

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The electronic structures of carbon nanotubes are governed strongly on the diameter and chirality. Since the nanotubes are exposed to the surface, electronic structures are expected to be severely modified by environment such as solvent and adsorbates. Yet, the effect of solvent and adsorbates to the electronic structures of carbon nanotubes has been rarely investigated. In general, a charge transfer between adsorbates and carbon nanotubes occurs, therefore modifying the electronic structures of carbon nanotubes. By precisely understanding the charge transfer mechanism, one may engineer carbon nanotubes to be suitable for many applications in electronic devices such as transistors and transparent conducting films. We will discuss a method of precisely engineering p- and n-type doping.

18:30
Advances in the chemistry and applications of carbon nanomaterials

Robert C. Haddon
Center for Nanoscale Science and Engineering, University of California, Riverside

The ability to chemically modify carbon materials offers considerable scope for the control of their chemical and physical properties. I will discuss our recent work on the synthesis, purification, characterization and chemistry of single-walled carbon nanotubes, graphite nanoplatelets and graphene together with selected applications involving their use in electronic devices, detectors, sensors, fuel cell components and thermal interface materials.

19:00

Synthesis and characterisation of ultra-thin conducting carbon films

Georg S. Duesberg[1] Tarek Lutz[1] Shishir Kumar[1] Nick Whiteside[1] Gareth P. Keeley[1] Niall McEvoy[1]
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Two synthesis routes for Ultrathin conducting carbon layers (UCCLs) are undertaken: 1) catalyst free CVD deposition from carbon precursors and 2) annealing of resigns at elevated temperatures. Both ways yield planar UCCLs with thicknesses below 10 nm with a roughness below 1 nm. The layers are found to have conductivities up to 105 Sm, close to those of TiN or TaN, as well as recently published for large area graphene films. The CVD deposited pyrolytic carbon layers allow conformal filling of high aspect ratio structures. This combined with the possibility of residue free etching promises the integration with current silicon fabrication lines. For the pyrolysis resigns we employed in particular negative tone resists to directly structure the ultrathin conducting electrodes by optical and e-beam lithography. The layers have been characterised in structure and morphology and examples for integration are shown. The easy and economic fabrication techniques of UCCLs presented are major steps towards the use of carbon in VLSI applications such as conducting liners or gate electrodes, as well as flexible conducting electrodes for displays and solar cells.

19:30

Sensing mechanism behind the metal-decorated SWNT-FETs

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Metal decoration on single-wall carbon nanotubes (SWNT) have shown to be an efficient way to catalyze chemical reactions, improve field emission efficiency, and sensor performances. We show that metal-decorated SWNT field effect transistors can be used as biosensor platforms. Previously, metal cluster-decoration on SWNT sensors proven to give selectivity by catalytic reaction of Pd nanoparticles, and sensitivy enhancement was achieved by decorating Al nanoparticles. For biosensing applications, we use Au or Ni nanoparticles on SWNT as immobilization support for molecular recognition elements. Ni or Au nanoparticles were decorated on sidewalls of SWNT by electrochemical deposition, and we could control the size and density of nanoparticles by controlling different parameters such as sweep voltage, speed and metal salt concentrations. Thiolated probe DNA or peptide nucleic acid (PNA) can be covalently immobilized on Au nanoparticles, while his-tagged antibodies can be immobilized on Ni nanoparticles. Clear change of conductance observed upon immobilization and target binding, and we will explain those observed changes with

metal work function.

1
Pristine and intercalated single wall carbon nanotubes and graphite revisited: A key to graphene

Thomas Pichler[1] Christian Kramberger[1] Alexander Grüneis[1] Angel Rubio[2] Martin Knupfer[3] Roman Schuster[3] Denis Vyalikh[4] Sergey Molodtsov[4] Erik Einarsson[5] Shigeo Maruyama[5] Claudio Attaccalite[2] Lucia Reining[6] Christine Giorghetti[6] Ralf Halmbach[6] Jörg Fink[7] Rolf Follath[7]
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[7]BESSY II, Berlin, Germany

In this contribution an overview about our recent results on the electronic and optical properties of pristine and intercalated aligned single wall carbon nanotubes and graphite using high energy spectroscopy techniques, namely angle resolved photoemission and electron-energy loss spectroscopy, as probes is presented. The consequences of doping on basic correlation effects and local field effects and their influence on the band structure and the plasmon dispersion are discussed in detail. Especially, we will show the impact of our results in order to unravel the underlying electronic and optical properties of graphene. Work supported by the DFG projects PI 440 3/4/5.

2
Preparation and selective properties of a new composite material for electrochemical capacitor built of single-wall carbon nanotubes coated with the fullerene-palladium co-polymer and bithiophene polymer film

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A new composite material for charge storage in electrochemical capacitors was devised and tested. It was built of electrophoretically deposited HiPCO single-wall carbon nanotubes, non-covalently surface-modified by 1-pyrenebutiric acid (pyr-SWCNTs), and then coated by electropolymerization with a film of mixed fullerene-palladium (C60-Pd) and bithiophene polymers. Both the electrophoretic and electropolymeric deposition was in situ monitored by piezoelectric microgravimetry with an electrochemical quartz crystal microbalance. The AFM imaging of the material showed tangles of pyr-SWCNTs bundles surrounded by globular clusters of the (C60-Pd)-bithiophene polymer. The pyr-SWCNTs/(C60-Pd)-bithiophene film revealed two potential windows of electrochemical activity, i.e. one at potentials more negative than ca. -0.40 V vs. Ag/AgCl and the other at more positive than ca. 0.40 V, characteristic for the C60 moiety electroreduction and thiophene moiety electro-oxidation, respectively. Both cathodic and anodic currents for the pyr-SWCNTs/(C60-Pd)-bithiophene film were higher than those for the control (C60-Pd)-bithiophene film due to higher area and hence capacitance of the former film.

3

Raman Scattering and X-Ray Diffraction from Ferrocene Encapsulated in Narrow Diameter Carbon Nanotubes

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Filling carbon nanotubes (CNTs) with fullerenes is limited to diameters larger than 1.3 nm. We studied peapods prepared with ferrocene as filling species, which allows filling of CNTs with diameters down to 1 nm. Two different nanotube samples with mean diameters of 1.1 nm (HiPco) and 1.6 nm (DIPS) were used. Filling was done from the gas phase at elevated temperatures and in addition with supercritical CO_2. Sample analysis was done by multifrequency Raman spectroscopy and X-ray diffraction. The Raman response from the encapsulated molecule could be observed through the wall of the CNTs. In X-ray diffraction filling was concluded from a loss of diffraction intensity from the bundle peak and from the appearance of a chain peak. Raman spectroscopy and X-ray diffraction independently confirmed the encapsulation of the employed molecular species. After heat treatment of ferrocene filled HiPco tubes several high frequency Raman lines were observed in the radial breathing mode frequency range which are ascribed to the Raman response from very thin inner shell tubes with diameters down to 0.4 nm. This work was supported by the FWF project I83-N20 (ESF IMPRESS).

4

Resonant Raman spectra of graphene with point defects

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We calculated the Raman spectra of graphene with a mono-vacancy, a di-vacancy, and a Stone-Wales defect using a non-orthogonal tight-binding model. We found that the presence of defects modified the band structure of graphene resulting in essentially resonant Raman scattering from phonons in the visible range. We analyzed the characteristic Raman-active phonons and their resonance energies for each defect. In particular, the introduction of di-vacancy and Stone-Wales defects in graphene makes the Raman scattering from the G-mode resonant in the visible range. This reason for resonant enhancement should be taken into account along with other well-established mechanisms, such as double-resonance scattering.

5

Raman detection of the Kohn anomaly in the K-point derived region of the Brillouin Zone of metallic carbon nanotubes upon electrochemical doping

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We applied Raman spectroscopy to investigate the response to electrochemical doping of the second-order D* band in single-walled carbon nanotube (SWNT) bundles. Our study reveals a dramatic increase of the D* band sensitivity to doping upon moving the laser excitation to the red end of the visible spectrum and beyond. We interpret this phenomenon as a confirmation for the existence of a second Kohn anomaly in the K-point derived region of the Brillouin zone (BZ) of metallic SWNTs, which stems from the Kohn anomaly in the K-point of the BZ of graphene. Our results are thus comparable to those of doping experiments on graphene by means of field-effect gating, and can be used to investigate the electron-phonon coupling in the bulk of the BZ of metallic SWNTs.

6

Transition Metal Nanoparticles by Urea Decomposition and Co-Precipitation Methods for CNT Growth

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Metal nanoparticles to be used as catalysts in bulk production of carbon nanotubes (CNTs) by chemical vapour deposition (CVD) have been prepared by a wide variety of techniques. In this work we synthesized nano-size metal catalyst powders by hydrothermally treating metal nitrates and chlorides (nickel and cobalt)

with the addition of urea or sodium hydroxide followed by calcination to induce oxidation. The powders were then reduced at high temperature in hydrogen gas to get nano-size particles. The effect of precursors used and preparation methods on the crystal structure and morphology of the obtained metal nanoparticles has been investigated. The co-precipitation method performed by using metal chlorides with sodium hydroxide gave rise to nanoparticles with uniform size. On the other hand, by using metal nitrates and urea, the particles are non-uniform in size. Catalysts have been characterized by XRD and SEM. These powders were then used to grow CNTs by alcohol CVD. A discussion comparing the yield and quality of nanotubes obtained by this process depending on the catalyst preparation method is reported.

7

High speed carbon nanotube memory elements

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Single-walled carbon nanotube field-effect transistors (CNT-FETs) are demonstrated to have impressive device parameters. They are extremely fast having a transit frequency as high as 50 GHz and have high sensitivity in monitoring single-electron tunneling events between a gold particle and a nearby nanotube. These CNT-FETs display often some degree of hysteresis in their transfer characteristics. For a transistor this is an unwanted attribute but it opens up new possible applications. By utilizing this hysteresis, CNT-FETs can be used as a memory element. The insulator film between the gate and CNT has here a crucial influence on the operation of the CNT-FET. For an effective capacitive coupling between the CNT and the gate electrode, a thin and dielectrically strong film is required. On the other hand, in order to achieve the desired hysteretic behavior for memory operation, the gate-CNT coupling has to include charge traps within the gate insulator or at some interface in the system that can be filled or emptied with charges from the CNT.

Here we will present the results on a first high performance charge trap CNT memory element with operation speed below a microsecond regime.

8

Stable colloidal Co-Pd nanocatalysts for carbon nanotube growth

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The standard way to make catalysts for surface-bound growth of carbon nanotubes is to evaporate or sputter the metal catalyst (Fe, Ni, Co..) onto the surface.

A lower cost method for large areas is to use liquid delivery. Colloids have the advantage of containing the catalyst in nanocluster form. Our previously developed colloids worked, but had a limited shelf-life due to oxidation and coagulation problems. Here, we have developed an air stable Co-Pd colloidal catalyst which works and has a long shelf-life.

9

Multi-Component Catalysts for the Synthesis of SWCNT

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We developed a large-scale synthesis of single-walled carbon nanotubes (SWCNT) based entirely on the electric arc evaporation method. To get the desired result, an enhanced understanding and control of the evaporation process is of crucial importance. For best results, one has to control the temperature gradient of the evaporation zone for a high evaporation density (difficult task) â or alternatively â one has to develop catalysts suitable for catalytic operation over a large temperature range. We found catalyst systems that allow both a low temperature-SWCNT-growth (200○C) as well as a high-temperature growth (1000○C). We also found a direct relation of the nanotube defect density on the choice of catalyst. In both cases multi-component catalysts offered the best results (large synthesis temperature range, low defect density, high yield).

10

Electrophysical properties of multiwalled carbon nanotubes with variable diameters

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Multiwalled carbon nanotubes (MWNTs) were produced via CVD method. Variation of catalyst composition and reaction conditions allows to produce MWNTs with controllable and relatively narrow diameter distribution. We have investigated temperature and magnetic field dependences of conductivity of MWNTs with different mean diameter using four-point probe technique in the temperature range 4.2 K - 300 K and in the magnetic field up to 6 T. Our previous researches of powder MWNTs carried out by this method showed stability and reproduci-

bility of results of the conductivity measurements. Only quantum corrections for interaction electrons (QCIE) in quantum corrections to magnetoconductivity take place, It was attributed to the absence of the bulk formations of amorphous carbon in MWNTs produced. From the data of QCIE we have estimated the constant of electron-electron interaction which is negative and monotonically falling with decrease of the mean diameter of MWNTs. This result is in opposite with experimental observation of superconducting state in SWNTs but in good agreement with data for MWNTs. Influence of NT defectiveness and structure on NT electrophysical properties is discussed.

11

Molecular Dynamics Simulations of Picotube Peapods

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Carbon picotubes are a promising starting point for the specific synthesis of nanotubes. In this context the interaction between nanotubes and picotubes is of particular interest. One potentially useful configuration evolves from inserting picotubes into a nanotube in a row in analogy to fullerene peapods. We perform temperature-dependent molecular dynamics simulations on such a system consisting of three tetramer picotubes arranged along the axis of a (9,9) nanotube. Covering a temperature range from room temperature up to 3000 K we observe two remarkable effects: First, our studies clearly show a directional transport of the tetramer molecules through the nanotube. Moreover, at sufficiently high temperatures breaking and formation of new bonds results in a structural reorganisation, which under suitable conditions might yield a second, inner nanotube of defined chirality.

12

Numerical usage of line group theory in the identification of Raman active modes in phonon spectra of single walled carbon nanotubes

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Calculating the phonon spectrum of an arbitrary single walled carbon nanotube becomes cheap in numerical sense, by exploiting the screw axis symmetry. The eigenvectors of the dynamical matrix are the irreducible basis vectors of the representation of the symmetry group of the nanotubes: $\mathbf{L}\left(2n\right)_n/mcm$ for achiral and $\mathbf{L}q_p22$ for chiral tubes. We developed a numerical code that solves the eigenvalue problem of the dynamical matrix produced by a DFT code (VASP), in the helical Brillouin zone. The code represents the symmetry elements of the line group on the $3N$ dimensional space, where N is the number of the carbon atoms in the helical unit cell. After decomposing the matrix representation we obtain one to one correspondence between the vibrational modes and the irreducible representations of the line group. The method allows to determine the frequencies of Raman-active and infra-active modes for any single walled carbon nanotubes.

13

Graphene flake detection with optical microscopy

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The graphene properties have already attracted the attention of scientists. The graphene flakes after their formation should be positioned onto semiconductor surface and identified with an optical microscopy for their further studies. In this work we present a modeling of the light beam passage through a three layer system „graphene-thin film-silicon“and a calculation of the graphene vision contrast dependence on the incident light wavelength. A refractive index and a thickness of the thin film were varied in this work. As a conclusion a material being transparent in a visible spectral range with the refractive index ranging from 2 to 2.2 should be chosen for the best graphene layer. From the list of appropriate materials ZnS and ZrO2 have been chosen for our experiments together with SiO2 due to their availability. The graphene flakes were prepared by the micromechanical cleavage of HOPG and were deposited on silicon substrates covered with thin films of these materials of different thickness. A good adhesion and good contrast have been achieved. The films have been studied with the atomic-force microscopy and the Raman scattering techniques.

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Rethinking carbon nanotube growth modes

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The technological possibilities harnessed by carbon nanotube (CNT) devices and materials have resulted in a worldwide anticipation of unprecedented advances in the realm of molecular electronics and smart materials; however, the true potentials of carbon nanotubes are yet to be unleashed. One of the main reasons for this is the lack of control in growing carbon nanotubes. Despite many studies centered on their synthesis, our understanding of the fundamental patterns involved in their nucleation and growth processes remain somewhat limited. In this presentation, studies of carbon nanotube growth using floating catalyst synthesis routes (laser evaporation and arc-discharge) are presented alongside chemical vapour deposition (CVD) routes using catalyst supports and gas phase prepared nanoparticles. The potential of ceramic based nanotube growth is also explored. These comparisons open up new opportunities to better understand the role of the catalyst particle since information on correlations between the initial catalyst nanoparticle and the engendered CNT are easily obtained. Data obtained on CNT nucleation and growth from the use of different supports suggests that a more stable growth process can occur from the ceramic support itself.

15

Spin Dependent Transport in ZnPc Single Layer Devices and C_{60}-ZnPc-Solar Cells

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We investigated ZnPc single layer devices and C_{60}-ZnPc-solar cells by means of continuous wave and pulsed electrically detected magnetic resonance (EDMR). Preliminary data [1] on ITO/ZnPc/Al structures are reviewed in the context of new results on coplanar Au/ZnPc/Au devices. Both samples exhibit the same current enhancement signal, when electron spin resonance is applied to it, indicating that there is no influence from the electrodes. A detailed phase analysis reveals two components of the signal with different line width but close resonance positions. Both components are attributed to the partners of a spin-pair involved in a spin dependent transport process. The similar g-values and the positive sign of the signal components lead to the assumption, that this process is rather a hopping than a recombination as assumed in [1]. First EDMR results on C_{60}-ZnPc-solar cells reveal two signals different in sign and line width. One of them is identical to the ZnPc-signal, the origin of the second one is still unclear.

[1] S. Schaefer, S. Saremi, K. Fostiropoulos, J. Behrends, K. Lips, and W. Harneit, Phys. Stat. Sol. (b) 245, Issue 10, (2008), 2120

16

MODELING OF CHEMICAL PROCESSES IN THE LOW PRESSURE CAPACITIVE RADIO FREQUENCY DISCHARGES IN A C2H2/Ar MIXTURE

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The gas discharge in hydrocarbon mixtures is widely used for carbon film growth. Noble gases like argon and neon are often used as main background gases for hydrocarbon mixtures as their presence changes morphology of diamond like carbon films and leads to fewer crystalline defects. We consider the formation of heavy hydrocarbons in a capacitive 13.56 MHz discharge operating in a mixture of C_2H_2/Ar at a gas pressure of 75 mTorr. For simulation we developed a hybrid model which combines the kinetic description for electron motion and the fluid approach for negative and positive ions transport and plasmochemical processes. We found that a significant change of plasma parameters related to injection of 5.8 % portion of acetylene in argon was observed and analyzed. We found also that the electronegativity of the mixture is about 30 %. The densities of negatively and positively charged heavy hydrocarbons are sufficiently large to be precursors for the formation of nanoparticles in the discharge volume. We have also found that the cluster growth does not affect the electron density and mean energy, but the densities of positive and negative ions increase.

17

Tracking down the crystallographic etching of graphene at the atomic scale

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Recent research into the channeling of few layer graphene via catalytic hydrogenation using metallic catalyst nanoparticles shows that this technique is potentially a key engineering route for graphene nanoribbon fabrication with atomic precision. In this study we exploit the benefits of aberration corrected high-resolution transmission electron microscopy to gain insight to the hydrogenation process whose mechanism remains controversial to date. The etch tracks are found to be commensurate with the graphite lattice. More importantly, detailed analysis of the catalyst structure and morphology reveals that the catalyst particles at the head of an etch channel are faceted and the angles between facets are multiples of 30Â°. Thus the catalyst facets are also commensurate with the graphite lattice. Structural analyses of the catalyst particles from treatments in different atmospheres unveils that carbide phases are not present during the hydrogenation process. This furthers our understanding on the underlying mechanism at an atomic level.

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Electronic properties of alkali intercalated SWCNTs

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We study the electronic properties of SWCNTs intercalated with Li, Na, and K using electron spin resonance and Raman spectroscopy, and microwave conductivity. The samples are prepared by the conventional alkali evaporation method for K and in liquid ammonia solutions for Li and Na. The alkali doping level is monitored by Raman spectroscopy using the shift of the Raman G mode as it is sensitive to the transferred charges. The ESR signal, characteristic of conduction electrons develops upon the alkali intercalation. Its intensity directly measures the density of states (DOS) at the Fermi level. The experimental DOS for the highest doping level is compatible with the DOS calculated for an SWCNT assembly which establishes that the nanotube assembly behaves as a Fermi liquid.

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Polarisation dependent colour tuning by doping of self assembled Para-sexiphenyl nanostructures

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Organic small molecules have been object of extensive studies in the last decade due to their promising and actual applications in optoelectronic devices. Nevertheless, critical issues for the fabrication of devices like, optimization of the emission purity and improvement of the device efficiency, represent a broad spectrum of possible improvements. A recent approach to controllably tune the colour emission of organic materials makes use of an efficient non radiative energy transfer occurring between two suitable organic molecules.
We deposited self assembled Para-sexiphenyl (PSP) crystalline nano-structures doped with alpha-sexithiophene (6T) on mica substrates. Atomic Force Microscopy shows, that the over all morphology and orientation of the nano-fibres is not affected by the incorporation of 6T, suggesting a good alignment of the 6T molecules in the PSP lattice. By room temperature photoluminescence (PL) a Foerster energy transfer between matrix and dopant was observed. Moreover, a strong dependence of the PL intensity on the polarization of the excitation suggests a good coupling of the transition dipoles of 6T and PSP and allows a colour tuning of the PL emission.

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Temperature Dependence of Electrical Conductance in Graphene

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We measured the temperature dependence G(T) of electrical conductivity in monolayer graphene designed in the field effect transistor (FET) configuration. Instability and changes in the dependence G(T) during the heating-cooling cycles are found to be related to the mesoscopic conductance fluctuations, typically present in 2-dimensional disordered systems. The phase shift of the interfering electron waves can be tuned by the voltage applied to the gate of the FET device. We found that, as the phase coherence with heating is progressively destroyed, conductance fluctuations vanish slightly above 50 K. This explains why, in this low temperature range, significant changes of the G(T), either an increase or a decrease, are observed. At higher temperatures, the G(T) is determined by the charge density: In the vicinity of the charge neutrality point (NP), conductance increases with rising temperature; at high charge densities phonon scattering becomes dominant and conductivity decreases during heating up from 50 to 250 K. We believe that the observed conductance instability at even higher temperatures is due to the high mobility of the charge defects, enabling their redistribution.

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Shear-stimulated formation of carbon nanotube networks in polymer matrices

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We report on the effects of shear-induced network destruction and formation in MWNT-composite melts which were directly monitored by the time-resolved DC-conductivity measurements during steady shear. A small steady shear applied for 1 hour to a non-conductive composite with initially well-dispersed nanotubes was found to induce the insulator-to-conductor transition resulting in a conductivity increase by about 6 orders of magnitude. The shear modulus measured simultaneously decreased by a factor of 2. In the rest time after steady shear both the electrical conductivity and the shear modulus demonstrate an increase related to the re-formation of the network in a quiescent melt. For the modelling of the network formation a shear-dependent kinetic equation for the nanotube agglomeration was coupled with the effective medium approximation for insulator-to-conductor transition. The proposed model gives a good qualitative description of the shear-induced effects in MWNT-polymer melts. The interplay between the destruction and reformation effects seems to have a fundamental origin in the polymer matrices subjected to steady shear flows.

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Millimetre height carpet of carbon nanotubes produced by Chemical Vapor Deposition in the presence of water

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We have successfully synthesized forests of vertically aligned carbon nanotubes (CNTs) with millimetre heights by the water assisted Chemical Vapor Deposition process. The CNTs forest can be easily patterned into macroscopic organized structures with define shape. This open up new applications in nanoelectronics, switches and displays systems.

By proper tuning of the water amount, CNTs walls number and diameter as well as forests height and density are controlled. Indeed, the CNTs mechanical properties are enhanced likewise. CNTs Young moduli close to the ideal 1TPa have been measured. In addition, the growth temperature can be dramatically lowered by using catalyst made of transition metals other than Fe or binary metal alloys.

Finally, we performed parametric study in order to substantiate the role of water during the reaction and to question the hypothesis of Hata et al. [1] that water enhances the catalytic activity by etching the amorphous carbon deposited during the CVD process.

[1] K. Hata, D.N. Futaba, K. Mizuno, T. Namai, M. Yumura, S. Iijima. Science, 306, 2004, 1362.

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Raman study of double-walled carbon nanotubes under high hydrostatic pressure

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Since the development of high-yield synthesis of double-walled carbon nanotubes (DWCNTs), interest in this system has been increasing due to the superior properties of double- compared to single- and multi-walled nanotubes. In this study we use hydrostatic high pressure to probe structural stability and tune vibrational and electronic properties of bundled DWCNTs produced by C60 peapod conversion. Raman data demonstrate DWCNT stability up to 10 GPa, the highest hydrostatic pressure in our experiment. The RBM pressure derivatives, dw/dP, of the outer tubes are several times larger than those of the inner tubes - the former act as a protective shield for the latter upon pressure application while the inner tubes provide the structural stability to the outer ones [1]. We probed the response of the metallic outer tubes to high pressure and observed a gradual decrease of the FWHM of G-(BWF) component on pressure increase, indicating weakening of the electron phonon coupling. In addition, we observed anomalous behavior of G- and RBM mode frequencies above 4-5 GPa. Possible origins of this anomaly are discussed.

[1] D. Christophilos, et al. Phys. Rev. B, 76, 113402, (2007).

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Superconductive pumping of nanomechanical vibrations

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In a recent paper (Sonne et al. PRB, 78, 144501) we demonstrate that a supercurrent can pump energy from a battery that provides a voltage bias into nanomechanical vibrations. Using a device containing a nanowire Josephson weak link as an example we showed that a nonlinear coupling between the supercurrent and a static external magnetic field leads to a Lorentz force that excites bending vibrations of the wire at resonance conditions. We also demonstrated the possibility to acheive more than one regime of stationary nonlinear vibrations and how to detect them via the associated dc Josephson current. These topics will be presented together with possible applications of such a multistable nanoelectromechanical dynamics.

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Theoretical study of atomic and electronic structure of magnesium diboride single-wall nanotubes

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We systematically studied the energetic and the electronic structure of MgB_2 nanotubes with outer, inner and staggered configurations of magnesium atoms in the framework of the density-functional theory. It was shown that the energetic stability of MgB_2 tubes with outer and staggered magnesium layer displays minimum at certain diameters of the boron cage. We studied the influence of boron environment on energetic stability of MgB_x nanotubes of different compositions like MgB_3. Except narrow MgB_2-NT with outer Mg arrangement, for which the structural tension opens the band gap, the MgB_2 nanotubes display metallic properties.

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Characterization of On-Chip filling of CVD grown Carbon Nanotubes

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Because of their ballistic conductance Carbon Nanotubes (CNTs) are a promising material for electronic devices. Their transport properties can be altered by functionalization. This can be done by filling the inner hollow of CNTs with guest molecules like C_{60}. The on-chip filling is carried out in an evaporation chamber providing a dynamic vacuum and additional heating directly on TEM grids. Therefore individual CNTs can be observed during the different steps towards peapods synthesis using HRTEM measurements. But even at electron energies as low as $E_e = 80\,keV$ individual CNTs and especially C_{60} molecules are destroyed during electron irradiation indicated by the collapse of sidewalls and coalescence of interior C_{60}. Therefore, we use Raman spectroscopy as a non-destructive method to characterize CNTs during peapod synthesis and correlate these measurements with our microscopic results. We compare samples grown at different temperatures using chemical vapor deposition (CVD). For bulk samples we use FT-Raman, which provides a fast and easy method, while we use confocal Raman for individual tubes, which allows localized measurements on single CNTs.

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Fermi Level shift in C60 by interfacial interactions in bilayer structures

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C60 and derivatives are key electron acceptor molecules for organic device applications such as field effect transistors and solar cells. In this work we concentrate on bilayer structures involving C60. We study in detail two C60 â insulator heterojuctions [1]: C60 grown on Al2O3 and C60 grown on divinyltetramethyldisiloxane-bis(benzocyclobutene) (BCB). By electrical characterization of these two metal insulator semiconductor structures a difference in the build-in field of about 0.8 V is determined. The very same structures we investigated by means of photoemission

spectroscopy. It is clearly seen from the UV photoemission spectra, that the work functions and therefore the Fermi levels of the fullerene in these two structures differ about 0.8 eV. This shift in the Fermi level corresponds to the investigated change in the build-in field, demonstrating a way to influence device characteristics by modifying electronic properties. It is demonstrated that the introduction of a BCB layer enhances the organic transistor performance [2].

[1]W. Osikowicz, M. P. de Jong and W. R. Salaneck, Adv. Mater. 19, 4213 (2007)
[2]X.-H. Zhang and B. Kippelen, Appl. Phys. Lett. 93, 133305 (2008)

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Tunable few-electron double quantum dots and Klein tunnelling in ultra-clean carbon nanotubes

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Carbon nanotubes (CNTs) have several unique properties that make them highly attractive for studying the coherent properties of single spins. In particular, nuclear spins, the principal source of spin decoherence in GaAs, can be completely eliminated. Furthermore, a strong spin-orbit interaction recently discovered in CNTs enables all-electrical spin manipulation, while preserving long spin relaxation and decoherence times. To study single spins using quantum dots (QDs), a single electron must be confined in a QD with highly tunable barriers. In previous studies of tunable CNT QDs, disorder has prevented devices from reaching the single-electron regime. Here, we present a new device which incorporates multiple local gates with an ultra-clean suspended CNT. Using these gates, we confine, for the first time, a single electron and a single hole in a tunable double quantum dot. Interestingly, this tunability is limited by a previously unobserved type of tunnelling, analogous to that in the Klein paradox of relativistic quantum mechanics.

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Self-organized critical networks with gold nanoparticle vertices and conductive $Mo_6S_{9-x}I_x$ nanowire edges

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Scale-free self-organized critical networks are known to show resistance to failure, fast signal processing and are of particular interest for nanoelectronics. They are also the basis of information processing in the brain. Self-organized criticality has been recently observed on a molecular scale in $Mo_6S_{9-x}I_x$ (MoSI) and gold nanoparticle (GNP) hybrid networks.

Solution processed attachment of MoSI nanowires to GNPs was used for self-assembly of the networks, which were deposited onto mica substrate, examined by atomic force microscope and statistically analyzed. With conversion of the net-

work into a simplified topological graph we were able to perform detailed analysis on a large part of the network.

We have compared distributions of lengths of individual nanowires to the lengths of the edges in the network and while the former is log-normal, the latter shows a strong power-law tail exhibiting scale invariance. This shows that the self-organized critical behaviour is not a property of the nanowire synthesis, but of their self-assembly into networks.

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Enrichment of single (n,m)-SWNTs by combining selective polymer-wrapping and density gradient centrifugation in organic solvents

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Since it has not yet been possible to fabricate custom-made SWNTs with defined length, diameter, chiral angle and electronic type, the development of separation techniques is necessary for gaining homogeneous samples. We describe a procedure which allows the facile production of monochiral single wall carbon nanotube suspensions using selective dispersion with fluorenyl based polymers, followed by a density gradient centrifugation in organic solvents. Solutions containing only one (n,m) species with an enrichment up to 90 % were obtained by choosing the right combination of starting raw SWNT material, polymer, ratio of polymer to SWNTs starting concentration, solvent and centrifugation conditions. Further tailoring of the (n,m)-distribution was then carried out by performing ultracentrifugation in a density gradient of tribromotoluene as density gradient medium in chlorobenzene. Evidence was provided by optical absorbance and photoluminescence excitation spectra.

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CARBON-SUPPORTED METAL NANOPARTICLES FOR H2 PRODUCTION

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Hydrogen has been extensively studied as the ultimate clean energy carrier to reduce air pollution and automobile emission. Ammonia decomposition producing COx-free hydrogen has attracted renewed interest due to its clean, sustainable and economical properties. Nano-sized Ru and Fe-Co clusters supported on carbon nanotubes (CNTs) are the most active catalysts, on which ammonia can be completely decomposed at low temperature. The graphitic structure of carbon support has been found to determine in essence the activity of metal nanoparticles. Nonetheless, the fundamental research is needed to reveal clearly the nature of reaction. Here we present our studies on the vital role of graphitic CNTs in decomposing NH3 into

H2 and N2. The structural and surface properties of catalysts were investigated by techniques such as TEM, SEM, EELS, XRD, Raman, TPSR, and so on. The in-situ synchrotron-excited XPS measurements at a near-ambient pressure reported direct evidences on the proposed electron transfer mechanism.

Reference: 1. J. Zhang, J.-O. Müller, W.Q. Zheng, D. Wang, D.S. Su, R. Schlögl, Nano Lett. 8 (2008) 2738â2743.

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Electrical properties of Palladium Functionalized Reduced Graphene Oxide

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The successful realization of applications based on nanostructures requires controllable tuning of their physical and chemical properties. Chemical modification is an attractive route to reach this task. Graphene, owing to its dimensionality, is expected to exhibit dramatic changes in its properties by its modification using appropriate chemical moieties. Here, we present the controlled modification of reduced graphene oxide layers by electrodeposition (and electroless deposition) of palladium nanoparticles and study its influence on the electrical characteristics. We further demonstrate that hydrogen sensitivity can be conferred onto individual graphene sheets by this modification process. Finally, we also show the influence of humidity on the electrical characteristics of both the modified and unmodified devices. The present work sheds further light on the physiochemical structure of chemically derived graphene which is not yet clearly understood.

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N-doped SWCNT film synthesis using a vertical flow aerosol reactor

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With the persisting challenge of controlling the electronic properties of carbon nanotubes (CNTs), doping with atoms such as nitrogen has been proposed as one viable solution. Pursuing this objective, we have employed a method to synthesize high quality N-doped single-walled CNTs, deposited as thin films directly from the gas phase in a simple continuous process. The ferrocene/CO/ammonia system used has been modified from [1].

The morphology, nitrogen doping concentration as well as the bonding configuration of N atoms in the carbon network have been resolved combining local and overall probes such as TEM, EELS and XPS. Some macroscopic properties of our films, such as sheet resistance have also been measured.

The work was supported by the EU (FP6 STREP project BNC-Tubes NMP4-CT-2006-03350).

[1] A.Moisala et.al, Chem. Eng. Sci. 61 (2006) 4393

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Carbon Nanotube Gates and Schottky Barriers in Carbon Nanotube Transistors

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The excellent mobility and electrostatic control of semiconducting carbon nanotubes (CNTs) and the high current carrying capability of metallic CNTs can be exploited in an all CNT based field effect transistor (FET). We have developed a method using two thermal CVD steps to produce doubly gated CNTFETs with a local CNT gate and a global back gate [1]. Transfer characteristics are in good agreement with results from theoretical simulations and give an inverse subthreshold slope of $S = 259$ mV dec$^{\hat{a}1}$ for the CNT gate and $S = 667$ mV dec$^{\hat{a}1}$ for the back gate sweep. The minimum gate delay is $\tau = 5$ ps at an I_{on}/I_{off}=100. Simulations show that $\tau = 2$ ps can be obtained if the thickness of the Si_3N_4 gate dielectric is reduced to 5 nm.

In addition the Schottky barriers at the Pd-CNT contacts have been studied using temperature dependent electrical measurements. The barrier heights decrease with increasing diameter of the nanotubes and they are in agreement with the values expected for little or no influence of Fermi level pinning.

[1] J. Svensson et al. *Nanotechnology*, **19**, 32520, 2008

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Electronic properties of carbon based nanostructures from GW calculations

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A general description of the electronic properties of model zig-zag carbon nanotubes (CNTs) and chiral-edge graphene nanoribbons using a new computational method for accelerating first-principles Green's functions calculations is presented. The electronic structures and the equilibrium geometries were obtained within the pseudopotential implementation of ab initio total energy DFT. Accurate calculations to determine quasiparticle excitations in carbon nanostructures, notably electronic band gap, are performed in the framework of the GW treatment of the self-energy. Good agreement with previous theoretical results on band gap of the (8,0) carbon nanotube at Gamma point and new model calculations on nanoribbons with edges irregularities show the potential of this method to perform accurate calculations on carbon-based systems of technological interest, otherwise difficult to address with conventional approaches. Furthermore, this technique may be used as a predictive tool of spectral properties, excited states and optical response of carbon based materials in extended systems.

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Expansion of graphite oxide lattice due to high pressure induced water insertion.

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Expansion of structure upon compression is a rare phenomenon that has been observed in composite systems due to incorporation of liquid pressure transmitting media into nanopores. A new type of anomalous pressure dependence of the unit cell volume is found for graphite oxide. The interlayer spacing of graphite oxide pressurized in the presence of water continuously increases by an extraordinary 28-30 percents with a sharp maximum at 1.3-1.5 GPa [1]. The increase of unit sell volume upon pressure increase is explained by incorporation of water into the interlayer space of the graphite oxide structure. The change from ânegativeâ to positive compressibility at 1.4 - 1.5 GPa coincides with the solidification of liquid water

into ice VI. At the same moment, the buckled graphene layers are stretched and slightly expanded laterally. The maximum of interlayer spacing was also observed during decompression at the point of ice melting. [1] A.V. Talyzin et al, Angew. Chem. 2008, 120, 8392 â8395

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High-Yield Separation of Metallic and Semiconducting Single-Wall Carbon Nanotubes by Gel Electrophoresis

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We have developed a novel separation method of metallic and semiconducting single-wall carbon nanotubes (SWCNTs) using agarose gel electrophoresis (1). When the SWCNTs were isolated with sodium dodecyl sulfate (SDS) and embedded in agarose gel, only the metallic SWCNTs separated from the starting gel by an electric field. After 20 min, almost all SWCNTs applied to gel electrophoresis were separated into two fractions, containing 95% semiconducting and 70% metallic nanotubes. The difference in the response to the electric field between metallic and semiconducting SWCNTs can be explained by the higher affinity of semiconducting SWCNTs to agarose than to SDS. In this presentation, we will also show the improved methods for the separation.

This study was supported by the industrial technology research grant program of the New Energy and Industrial Technology Development Organization (NEDO) of Japan. (1) T. Tanaka et al., Appl. Phys. Express 2008, 1, 114001.

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The anomalous behaviour of the ν_1-band of β-carotene in solution and within Photosystem I and II

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One of the most important pigments in photoactice proteins like photosystem I and II in higher plants is β-carotene, which in addition to its light absorbing ability also serves a protective function within the proteins due to its abilitiy to quench chlorophyll triplet states in order to prevent the formation of highly reactive singlet oxygen.

Raman spectra and Raman excitation profiles (REPs) of β-carotene are presented and compared with Raman spectra and REPs of Photosystem I and II excited in the Soret region. Main focus is the vibrational ν_1-band around 1500 cm^{-1}, which originates from the ground-state in-phase double bond C=C stretching mode of the isoprene units forming the backbone of β-carotene. The band consists of two unresolvable peaks possessing different resonance excitation profiles leading to an anomalous wavelength dependent shift of the band.

Theoretical approaches trying to explain this behavior are discussed like different Frank-Condon enhancement of the two modes due to different excited-state displacements of the vibrational modes or Duschinsky rotation, which describes intensity changes of resonance excitation profiles due to mode mixing.

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Thermal Expansion Co-efficient of Nanotube-Metal Composites

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Abstract: Thermal Expansion exhibits considerable challenges developing residual stresses in the interfaces of different materials treated at high temperatures, especially, the electrical devices often containing materials with different thermal expansion behaviour. Thermal expansion co-efficient (TEC) of different metals can be tuned by using carbon nanotubes (CNTs). Metal matrix composites (MMCs) using CNTs are fabricated by hot-press sintering method and thermal expansion co-efficient of different metals and alloys are investigated throughout wide range of temperatures (-155Â°C to 255Â°C). Reduction of TEC of the composite materials was observed up to 20% compared to that of pure metals. The effect of CNTs in the matrix materials and the mechanism behind the improvement are explained from the microscopic investigation of the composites.

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Long-term adsorption of fetal bovine serum on H/O-terminated diamond studied in situ by atomic force microscopy

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Diamond is an attractive material for biological systems due to its unique chemical and biological properties [M. Kalbacova et al. PSS(b) 245 (2008) 2124]. Here, we investigate adhesion of fetal bovine serum (FBS) on CVD monocrystalline diamond which has microscopically patterned regions of H- and O-termination. The diamond surfaces are processed photo-lithographically and by hydrogen (1200 W, 800 C, 10 min) and by oxygen plasma (300 W, RT, 3 min) to generate alternating

H/O-terminated patterns of 30 μm width. The samples were immersed into 15 % FBS in McCoy's 5A supporting medium and characterized by in situ atomic force microscopy (AFM) during 1 week. After one day 2-4 nm layer was formed on both H/O-terminated surfaces. After one week we observe 17 ± 5 nm FBS layer on O-terminated surface and 35 ± 5 nm on H-terminated surface. A protein depletion region of 2-3 μm width is observed at the boundary. Based on the above characteristics we present a model of FBS protein layers on H/O-diamond and we draw conclusions for a microscopic control of the protein-mediated adsorption and cultivation of cells in diamond-based implants and biodevices.

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AFM induced electrostatic charging of nanocrystalline diamond on silicon

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Electrostatic charging is widely used in a variety of technologies and devices. Diamond as a wide band-gap semiconductor is an interesting material for such applications (Čermák et al., Phys. Stat. Sol. A 205 (2008) 2136-2140). Here, AFM is used to induce electrostatically charged microscopic areas on nanocrystalline diamond (NCD) films of 80 nm thickness terminated by oxygen atoms. The films are deposited on silicon substrates. We study amplitude and spatial flucttutations of the stored charge as a function of AFM tip bias voltage and scan speed. For instance, we show local electrical potential differences up to -1 V using -20 V bias. We discuss contribution of diamond bulk and grain boundaries to the charging effects. We compare the results with charging of the silicon substrate itself as well.

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High-density Arrays of Carbon Nanotube and Graphene Devices: Directed Assembly and Rapid Characterization

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First, I discuss the fabrication of high-density arrays of single-chirality-SWCNT [1] and graphene [1] devices. We have shown that dielectrophoresis can be used to fabricate arrays of SWCNT devices, and the process is self limiting to one nanotube per device. [2] Single-chirality SWCNT suspensions are obtained by selective polymer wrapping and density gradient ultracentrifugation. Graphene solutions are made by exfoliating graphite in aqueous and organic solvents. The yield and quality of devices from a variety of suspensions is compared. Arrays are characterized by spatial Raman and photoluminescence maps and electron transport measurements.

Next, I present Voltage-Contrast Scanning Electron Microscopy (VC SEM) as a new technique for the rapid, parallel and visual electronic characterization of SWCNT devices. VC-SEM is shown to distinguish metallic and semiconducting SWCNTs in the SEM. [3] VC-SEM is also used to characterize defects, [1] such as Stone-Wales defects, high-current breakdown, e-beam induced metal-insulator transition and charge-injection into the dielectric substrate. (1) Unpublished/Submitted (2) Nano Letters 2007, 7, 1556-1560 (3) Nano Research 2008, 1, 321-332

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Structural properties of MoS2 „mama“– tubes and related materials

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MoS2 nanomaterials synthesized by sulphurization of Mo6S2I8 nanowires were studied by wavelength dependent Raman spectroscopy, XRD and HRTEM. The transformation process, determined by the reactor temperature, leads to selective morphologies of the MoS2, like coaxial nanotubes, i.e. nanotubes with split walls, „mama“-tubes, encapsulating MoS2 fullerene-like particles,[1] or other hybrid nanostructures. Temperatures above 850∘C lead to formation of MoS2 „mama“âtubes, while below 850∘C the growth of coaxial MoS2 nanotubes is favored. HRTEM was used to study how MoS2 layers form from outside of precursor nanowires to inside and to observe the nucleation of fullerene-like particles. Results of a possible oxidation during the Raman experiment are correlated with partially or fully oxidized Mo6S2I8 nanowires of the composition MoO3-x, which can be afterwards also sulphurized resulting in MoS2 polycrystalline nanowires. Using Raman and XRD spectroscopies we have studied effect of temperature and duration of the sulphurization process. We followed stages of the transformation to study the chemical reaction kinetics. [1] M. Remskar, A. Mrzel, M. Virsek, A. Jesih Adv. Mater. 2007, 19, 4276

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First principles studies of carbon nanotubes growth

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Controlling the chirality of CNTs is one of the obstacles of using them in electronic devices. It is crucial to fully understand their growth mechanism. Combining the idea of chemical vapour deposition and root growth model, we investigated the effects of different catalysts on the growth of single-walled CNTs by first principles calculations. Our first model compared different caps of the CNTs placed onto the

(111) surface of Ni, and compared their binding energies after relaxation. [1] Here we modelled various caps on the (111) surfaces of Fe, Co, Au, Mo, Ti to see the effects of other catalysts. We find that for all metal surfaces, the energy of the carbon-metal bonds for the armchair edges is 30% higher than for zigzag edges. As a more realistic model, we used a Fe nanoparticle of 55 atoms with three facets on which the caps are placed. Our results showed that the binding energy depends largely on cap diameter. Caps with diameter comparable to the facets are favoured. Facets with a pyramid tip are favoured and more stable bonds are formed.

[1] S. Reich et al. Chem. Phys. Lett. 421 (2006) 469

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Stability and Aromatic Structure of Graphene Nanoribbons

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We analyze the stability, the geometry, the electronic and magnetic structure of hydrogen-terminated graphene-nanoribbons edges as a function of the hydrogen content of the environment by means of density functional theory. Antiferromagnetic zigzag ribbons are stable only at extremely-low ultra-vacuum pressures. Under more standard conditions, the most stable structures are the mono- and di-hydrogenated armchair edges and a zigzag edge reconstruction with one di- and two mono-hydrogenated sites. At high hydrogen-concentration “bulk” graphene is not stable and spontaneously breaks to form ribbons, in analogy to the spontaneous breaking of graphene into small-width nanoribbons observed experimentally in solution. The stability and the existence of exotic edge electronic-states and/or magnetism is rationalized in terms of simple concepts from organic chemistry (Clar’s rule).

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Interplay between Kondo and Josephson Effect in a Carbon Nanotube Quantum Dot

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We present detailed transport measurements on single walled Carbon nanotube quantum dots coupled to superconducting electrodes. For intermediate transpa-

rency contacts, we observe various manifestations of the Kondo effect with the electrodes in the normal state, that also affect the superconducting state. Here, we observe a striking even-odd effect, visible in the subgap structure of nonlinear transport data, with the Andreev reflexion process at $V = \Delta/e$ being strongly enhanced in charge states with odd occupation. As an explanation we suggest the formation of a one-sided Kondo resonance on the more transparent one of the two contacts.
A Josephson current will get strongly modified in the presence of Kondo correlations. For for values of the Kondo temperature $T_K \leq \Delta$ the sign of the supercurrent is usually reversed, and the system is in the so called π-state. We show measurements of the Josephson current in several Kondo-states, where we can tune the Kondo-temperature with the resonant level position. This permits us to investigate the transition into the π-state, and to compare out data to recent functional renormalization group (FRG) calculations.

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Locally Gating via Trigates on a Single Germanium Nanowire

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Germanium is a well-known semiconductor from the early days of semiconductor industry. We use germanium as core element in the form of nanowires, as possible pathway for the semiconductor industry beyond the silicon era in order to fulfill Moore's law. Key-point of any electronic device is that the electrical transport properties are tuned with a nearby gate. As far as germanium nanowires are used as core element, the natural oxidation of germanium is a problem, preventing electrical contacting for charge-injection. In our contribution we make use of the germanium oxide, and turn this disadvantage into a benefit. We use this natural germanium oxide as a gate oxide, and we deposite metal trigates on a germanium nanowire. This approach should allow to tune the electrical properties locally along the Germanium nanowire. The impact of the trigate is probed by electrial transport measurements and presented in this contribution.

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Reaction-limited growth of single-walled carbon nanotubes

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We present a systematic study of the temperature dependence of the growth rate of vertically aligned multi-walled carbon nanotubes by thermal chemical vapor deposition of acetylene in the temperature range $560 - 800$ °C. We use Al_2O_3-supported

Fe particles as catalyst and C_2H_2 as feedstock. Growth is performed at atmospheric pressure. We also record the growth of carbon nanotube forests by high resolution real-time optical imaging. We derive activation energies of < 1 eV.

Carbon nanofibres and large diameter carbon nanotubes in PECVD are known to grow by diffusion limited growth, as their growth rate varies inversely with the catalyst droplet diameter. We also look at the pressure dependence of the growth rate of SWNTs and small diameter MWNTs in the C_2H_2 pressure (p) range of 10^{-5} to 20 mbar. We observe a $\sqrt{p}$ dependence. Thus, we suggest that the rate limiting step for SWNT growth under purely thermal conditions is molecular dissociation at the catalyst surface.

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Quantitative Evaluation and Control of the Diameter of Vertically Aligned SWNTs

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To quantify the diameter change along a vertically aligned single-walled carbon nanotube (SWNT) array grown by alcohol catalytic CVD, we compare three samples that followed almost the same growth curves but grew for different CVD time. By subtracting UV-Vis-NIR absorption spectra from each other, we obtain the local absorption information, which clearly show that the average diameter of SWNTs along a vertically aligned array is around 10-20% larger at the root than at the tip. The increase of diameter begins from a diminishing of signal in small diameter range and then a shift of the entire peak. From this observation, we discuss that catalyst aggregation is the main reason of the diameter increase rather than the catalyst ripening. Higher concentration of Mo is introduced into the original catalyst recipe to prevent from the aggregation of metal particles at high temperatures. As expected, the average diameter of SWNT arrays is significantly reduced. Small-diameter vertically aligned SWNTs (average diameter of 1.2 nm) have less buckling due to higher flexibility, which lowers the resistance of thermal and electric transport.

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Origins of optical absorption components of metallic and semiconducting single-wall carbon nanotubes in ultra-violet region

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There are large absorption components in the optical absorption spectra of single-wall carbon nanotubes (SWCNTs) in the ultraviolet (UV) region ($\sim$ 5 eV). Clarification of the origins of the UV absorption is important, since the tails of the UV components influence the transparency of nanotubes and impede their uses for transparent conducting films. However, the origins have still been under discussion. Such UV absorption components are assumed to be caused by π-plasmons. However, recently contributions from π-π^* transition at the M point were also suggested. To understand the origins of UV component in detail, here we clarified how the electronic structure (metallic or semiconducting) and the diameters of SWCNTs influence the UV optical absorption features. We clearly identified two components in UV region, and revealed dependence of the components on their diameters. Remarkably, dependence of the peak-energies of one component on diameters could not be explained by plasmon model, implying the presence of different origins than plasmons in the UV absorption components.

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Carbon Nanotube Composites Produced by Coagulation Spinning

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Surfactant-dispersed single-walled carbon nanotubes (SWNTs) were injected into a laminar flow of aqueous polyvinyl alcohol (PVA) to produce nanotube gel fibres, which were collected in a water bath on a spindle. An extensive study was carried out to optimise the polymer-SWNT-surfactant coagulation system. Various surfactants and a large number of PVA and surfactant injection speeds were used to find the optimum spinning conditions. A range of nanotube mass-fraction fibres were produced at these optimum spinning rates and the best fibres were drawn by various amounts; their mechanical properties were investigated by tensile testing. The resulting fibres had ultimate tensile strengths of up to 1.7GPa. Water absorption and induced crystallinity effects were also investigated.

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Synthesis of Carbon Nanotubes on Cobalt Disilicide for Horizontal Interconnect Application

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We identified Cobalt Disilicide (CoSi2) as a new electrically conducting material that can support vertically aligned Carbon Nanotubes (CNTs) growth. Compared with other conducting catalyst support materials (e.g. TiN and TaN), AFM study shows that CoSi2 has better thermal stability under our CNT growth condition (at

490-650C). It is also revealed that CoSi2 supported Fe catalyst particles do not undergo observable agglomeration upon pre-growth thermal treatment under H2 flow for 15 minutes, which largely outperforms SiO2/Fe and is comparable with that of Al2O3/Fe. We further show that Single-walled CNTs (SWNTs) can be grown with CoSi2/Fe at 700C in a cold wall system, the sample shows Radial Breathing Mode peaks under Raman Spectroscopy and hence confirms the presence of significant amount of SWNTs in the CNT forest.

With a Horizontal Growth Test Structure(HGTS), which has a 20 nm self-aligned CoSi2 layer on the vertical surface of electrode, we investigated the possibility of growing horizontally aligned CNTs from Fe catalyst deposited on such a vertical surface for the purpose of horizontal interconnect application.

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Commercial Carbon Nanotubes as Efficient Catalysts for Alkene Synthesis

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We herein report a facile and sustainable route to synthesize the alkenes as important monomers in modern polymer industries. After simple modification, the commercial CNTs efficiently catalyze the reaction under a mild condition. Tubular structure keeps intact during the whole process (1). This study will renew scientific and technological interests on large-scale applications of CNTs. Oxidative dehydrogenation of butane is an energy-saving technology to synthesize butenes and butadiene. The development of transition metal-based catalysts has been hindered by the big challenges in both selectivity and long-term stability. By using metal-free CNTs as catalysts, we were delighted to observe a high selectivity during a continuous reaction over 100 hours. At a same conversion of butane, surface-modified CNTs are much more selective than the well-developed V-Mg-O catalysts. The metal-free mechanism is well confirmed by both in-situ characterizations and DFT calculations. The application of CNTs as a heterogeneous catalyst is attractive due to the favorable management of energy.

Reference: 1. J. Zhang, X. Liu, R. Blume, A.H. Zhang, R. Schlögl, D.S. Su, Science 322 (2008) 73â77.

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Nanoelectromechanical quantum pumps formed of double walled carbon nanotubes

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Recently it was shown experimentally by the group of A. Zettl that nanomechanical devices comprised of a long stationary inner carbon nanotube and a short slowly

rotating outer tube can be fabricated [1]. In this work, we study the possibility of using such devices as adiabatic quantum pumps [2]. Using the recursive Green's function method (employing the Brouwer formula) we calculated the pumped charge from one end of the inner tube to the other, as driven by the rotation of the outer nanotube, studying a large number of different chiralities.
The Hamiltonian was described by the inter-molecular Hückel model, and for a few test cases by density functional theory. We have found good agreement between the two methods. Our results on the pumped charges show that there is virtually no pumping if the chiral angle of the two nanotubes is the same, as expected. We discuss which are the optimal chiralities that can be used for such quantum pumps. Furthermore, we show that charge pumping with such devices can be used to probe the strength of the inter-layer coupling between the inner and outer tube.
[1] Nature 424, 408 (2003)
[2] PRL 87, 236601 (2001)

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Opto-electronic performance of PPV-based heterostructures evaluated by scanning probe techniques

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It is believed that the low power conversion efficiency of organic solar cells (6%) is caused by imperfections in micro-structural ordering of the heterojunction [ÄermÃ¡k et. al., Phys. Stat. Sol. RRL 1 (2007)]. Thus microscopic characterization of their properties is of key importance for further development. Here, organic heterojunctions are prepared by spin-coating onto ITO covered glass substrates using PPV-based conjugated polymers. Microscopic morphologies of the organic films are studied by Atomic Force Micrscopy (AFM). Microscopic inhomogeneities of surface potentials (detected by Kelvin Probe Microscopy - KPM) and their different shifts under illumination indicate spatial variations of the carrier photogeneration. This is in a good agreement with the results obtained by photoinduced surface potential decay technique. Similar results are also observed by microscopic current-voltage characteristics measured via AFM tip in dark and under illumination. Micro-Raman mapping corroborates these data by revealing different degree of local phase separation. Some areas are even no more of heterostructural nature and therefore can lead to electrical shunting of the cells.

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Single walled carbon nanotubes modified by PFO -â An optical absorption and Raman spectroscopic investigation

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In this contribution we present preliminary results on the optical absorption and resonance Raman spectroscopic investigations on singlewalled carbon nanotubes (SWCNT) functionalized by poly (9,9-dioctyfluorenyl-2,7-diyl)-co-bithiophene (PFO). A route for a stable suspension of SWCNT in a solution of fluorene-based copolymer is shown. Additionally, the detailed analysis of the supernatant and the sediment after centrifugation of the functionalized sample is given. The resonance Raman and optical absorption spectroscopic data suggest the selective wrapping of carbon nanotubes by PFO occurs. Thus, the presented functionalization route is attractive as a means to separate semiconducting and metallic SWCNT.

Transport and magnetic properties of carbon nanotubes

8:30 – 9:00	N. M. Gabor, US *Highly efficient electron-hole pair generation via impact ionization in carbon nanotube p-n junction photodiodes*
9:00 – 9:30	D. Loss, CH *Nuclear spins in nanostructures*
9:30 – 10:00	V. Siegle, DE *Pumping single electrons with SWNT*
10:00 – 10:30	Coffee break
10:30 – 11:00	C. Boehme, US *Electrically detected coherent spin control in carbon based semiconductors*
11:00 – 11:30	B. Dora, DE *Electron spin resonance of Luttinger liquids and single-wall carbon nanotubes*
11:30 – 12:00	V. Krstic, IE *Doping of single-walled carbon nanotubes with phosphorous atoms*
12:00 – 17:00	Mini Workshops
17:00 – 17:30	E. Goovaerts, BE *Bile-salt solubilization offers high resolution and selectivity for the spectroscopy of single-wall carbon nanotubes*
17:30 – 18:00	E. D. Obraztsova, AT *Two-phonon Raman spectroscopy of one-, two-layered graphene and carbon nanotubes*
18:00 – 18:30	T. F. Heinz, US *IWEPNM09 – Conference summary*
18:30 – 20:00	Break
20:00	Bauernbuffet Farewell

Friday, March 13

8:30
Highly efficient electron-hole pair generation via impact ionization in carbon nanotube p-n junction photodiodes

Nathaniel M. Gabor[1] Zhaohui Zhong[2] Ken Bosnick[3] Jiwoong Park[4] Paul McEuen[1]
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[2]Department of Electrical Engineering and Computer Science, University of Michigan
[3]National Institute for Nanotechnology, National Research Council of Canada
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In carbon nanotubes (CNTs), the unique band structure leads to an effective fine structure constant $\alpha = e^2/(h/2\pi)v_F \sim 1$, where e is the electron charge, v_F is the Fermi velocity and h is Planckâs constant. $\alpha \sim 1$ suggests that electron and hole interactions, such as impact ionization, should be very strong in CNTs. Indeed, we observe highly efficient generation of electron-hole pairs due to impact ionization in carbon nanotube p-n junction photodiodes. To investigate optoelectronic transport properties of individual CNT devices, we scan a focused laser beam over the device at low temperature while monitoring the electronic characteristics. Optical excitation into the second subband E_{22} leads to striking photocurrent steps in reverse bias $I - V_{SD}$ characteristics at voltage intervals E_{GAP}/e. We attribute these steps to impact ionization and give evidence that E_{22} carriers efficiently ionize additional electron-hole pairs. In reverse bias, impact ionization leads to eventual avalanche breakdown, resulting in highly sensitive photon detection. Interestingly, evidence for electron-hole generation is observed even in forward bias, suggesting that CNTs may be an ideal building block for future photovoltaic technology.

9:00
Nuclear spins in nanostructures

Daniel Loss
Department of Physics, University of Basel, Switzerland

The physics of itinerant or quantum-confined electrons interacting with localized magnetic moments is central for numerous fields in condensed matter such as decoherence of spin qubits [1], nuclear magnetism [2-4], heavy fermions, or ferromagnetic semiconductors. Nuclear spins embedded in metals or semiconductors offer an ideal platform to study the interplay between strong electron correlations and magnetism of localized moments in the RKKY regime. In two dimensions the magnetic properties of the localized moments [2, 3] depend indeed crucially on electron-electron interactions. In one-dimensional (1D) systems such as single wall carbon nanotubes (SWNTs) electron correlations are even more important. For metallic (armchair) SWNT they lead to Luttinger liquid physics. Recently, SWNTs made of 13C, forming a nuclear spin lattice, have become experimentally available [5]. Motivated by this we have studied nuclear magnetism in metallic 13C SWNTs and showed that even a weak hyperfine interaction can lead to a helical magnetic order of the

nuclear spins coexisting with an electron density order that combines charge and spin degrees of freedom [4]. The ordered phases stabilize each other, and the critical temperature undergoes a dramatic renormalization up into the millikelvin range due to electron-electron interactions. In this new phase the electron spin susceptibility becomes anisotropic and the conductance of the SWNT drops by a universal factor of two.

W. A. Coish and D. Loss, Chapter in vol. 5 of the Handbook of Magnetism and Advanced Magnetic Materials, Wiley; cond-mat/0606550.

P. Simon and D. Loss, Phys. Rev. Lett. 98, 156401 (2007).

P. Simon, B. Braunecker, and D. Loss, Phys. Rev. B 77, 045108 (2008).

B. Braunecker, P. Simon, and D. Loss, arXiv:0808.1685.

H. O. H. Churchill et al., arXiv:0811.3236 (2008).

9:30

Pumping single electrons with SWNT

Viktor Siegle[1] Chen-Wei Liang[1] Sergey Lotkhov[2] Bernd Kaestner[2] Hans-Werner Schumacher[2] Florian Jessen[3] Dieter Koelle[3] Reinhold Kleiner[3] Siegmar Roth[1]
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[3]Physikalisches Institut â Experimentalphysik II, Universitaet Tuebingen

The ability of controlling the electrical current with high precision is of a great interest. Ultimatively, this requires to transfer a well-defined number of electrons per each time unit. Devices generating quantized charge current – so called single electron pumps or turnstiles – are broadly used in especially metrological applications.

We present a turnstile device based on individual SWNT or thin bundles contacted by superconducting (S) leads. Using the properties of the superconducting–normal-conducting interface in this hybrid S-SWNT-S design we are able to generate quantized charge current simply by applying RF-modulation at the back gate. The number of electrons transferred in each operation cycle is set by the RF-amplitude and can be controlled down to single electron level.

10:30

Electrically detected coherent spin control in carbon based semiconductors

Christoph Boehme[1] Dane McCamey[1] John Lupton[1] Kipp Van Schooten[1] Manfred Walter[1] Nick Borys[1] Sang-Yun Lee[1] Seo-Young Paik[1]
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Carbon based materials have an intrinsically weak spin-orbit coupling which imposes spin selection rules on many electronic transitions. The spin degree of freedom of electrons and nuclei can therefore play a crucial role for electronic and optical properties of these materials and these effects have been studied extensively with magnetic resonance related methods in the past.

This presentation is a review of the recently developed coherent (pulsed) electrically detected magnetic resonance spectroscopy (pEDMR). PEDMR allows the detection of coherently controlled spin-dependent electronic transitions through transient conductivity measurements. This approach provides a much greater sensitivity than conventionally detected magnetic resonance and it also allows the discrimination between paramagnetic centers which do influence conductivity and those which do not.

The presentation will review pEDMR as a method, its state of development, technical requirements and limitations, and discuss applications. Among them are spin-dependent transport in materials used for lighting (organic light emitting diodes) and photovoltaics for which these experiments help to gain an understanding.

11:00

Electron spin resonance of Luttinger liquids and single-wall carbon nanotubes

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A comprehensive theory of electron spin resonance (ESR) for a Luttinger liquid state of correlated metals is presented. The ESR measurables such as the signal intensity and the line-width are calculated in the framework of Luttinger liquid theory with broken spin rotational symmetry as a function of magnetic field and temperature. We obtain a significant temperature dependent homogeneous line-broadening which is related to the spin symmetry breaking and the electron-electron interaction. The result crosses over smoothly to the ESR of itinerant electrons in the non-interacting limit. These findings explain the absence of the long-sought ESR signal of itinerant electrons in single-wall carbon nanotubes when considering realistic experimental conditions.

11:30
Doping of single-walled carbon nanotubes with phosphorous atoms

Vojislav Krstić[1] Thomas Wågberg[2] Anne M. Janssens[3] Christopher P. Ewels[4] Odile Stéphan[4] Marianne Glerup[5]
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Doping of single-walled carbon nanotubes is a powerful technological tool to tune their electronic properties and thus has a wide impact on many fields of nanotechnology. We report on the proof and impact of doping of single-walled carbon nanotubes by incorporation of phosphorous atoms into the nanotube honeycomb lattice. The electronic properties of the doped single-walled carbon nanotubes are investigated by charge-transport, nuclear magnetic resonance and electron microscopy studies and underpinned by density-functional structural modelling. The phosphorous-doped nanotubes show a significant variation in tube morphology compared to their undoped counterparts going along with a non-Luttinger liquid like behaviour of the zero-bias conductance with additional irregular step-like features. A decrease and an inversion of the nuclear-magnetic-resonance relaxation times are observed suggesting metallic nanotube growth.

17:00
Bile-salt solubilization offers high resolution and selectivity for the spectroscopy of single-wall carbon nanotubes

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Solubilization of single wall carbon nanotubes (SWNTs) using surfactants [1] has by now become a standard preparation and characterization tool. Very high concentrations of isolated SWNTs can be obtained in aqueous solution using bile salts which also provide an only weakly disturbing environment for the nanotubes.[2] This yields major advantages in spectroscopy of SWNTs and of their nanohybrids with organic molecules. Increased resolution in Raman scattering allows for the selective detection of closed (empty) and open (filled) SWNTs by frequency shifts both of the vibrational radial breathing mode and of the electronic transition.[3] Also, nanohybrids of porphyrins adsorbed on SWNTs were studied by ESR and optical techniques, distinguishing between metallic and semiconducting tubes.[4] Quantitative techniques are proposed to determine the degree of opening of the nanotubes, and the fraction of metallic/semiconducting tubes.

[1] M.J. O'Connell, et al., Science 297 (2002), p.593; [2] W. Wenseleers, et al., Adv. Funct. Mater. 14 (2004), p.1105; [3] W. Wenseleers, et al., Adv. Mater. 19 (2007), p.2274; [4] S. Cambré, et al., ChemPhysChem 9 (2008), p.1930.

17:30

Two-phonon Raman spectroscopy of one-, two-layered graphene and carbon nanotubes

Elena D. Obraztsova[1] Ekaterina A. Obraztsova[1] Sofia N. Bokova[1] Alexander V. Osadchy[1] Rudolf Pfeiffer[2] Hans Kuzmany[2]
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According to calculations a number of graphene layers determine the electronic properties of graphene nanostructures being important for nanoelectronics and nanophotonics. A resonant Raman scattering (RS) is a tool being very sensitive to changes in the electronic structure. In this work we studied with RS graphene and carbon nanotubes with a small number of layers. The graphene has been produced by a micromechanical cleavage of HOPG [1]. The double-wall carbon nanotubes have been formed by a filling of arc single-wall carbon nanotubes with C60 molecules followed by a vacuum annealing at 1100 ∘C [2]. All samples have been studied first with HRTEM and atomic force microscopy. A main Raman feature under investigation was the two-phonon Raman band around 2700 cm-1. The differences in its position, shape, thermo-induced and resonant behavior for the flat and curved structures with the same layer number have been revealed. The experimental results almost have coincided with the computer modeling. [1]. E. A. Obraztsova et al., Phys. Stat. Sol. B 245 (2008) 2055. [2]. R. Pfeiffer et al. , Phys. Rev. B, 71(2005) 155409 (1-8). The work was supported with RFBR-07-02-01505, 07-02-91033AF

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