XXth International Winterschool

20th IWEPNM 2006

Euroconference
on
Electronic Properties
of
Novel Materials

Molecular Nanostructures

4. 3. - 11. 3. 2006

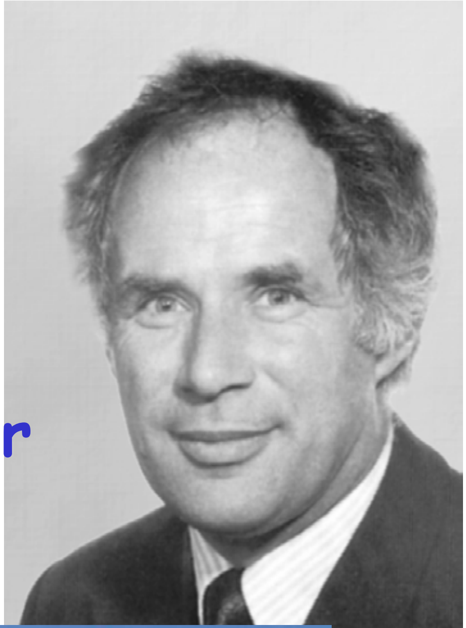
Hotel Sonnalp | Kirchberg | Tirol | Austria

IWEP NM 2006

SPECIAL ISSUE

PROGRAM

Hans



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Kirchberg, 4. 3. 2006

Ref.: International Winterschool on:
"Electronic Properties of Novel Materials: molecular nanostructures"
IWEPNM 2006, Kirchberg/Tirol, Austria

Dear Friend:

Welcome to the 20$^{\text{th}}$ International Winteschool on:
Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of nineteen previous meetings held in Kirchberg in the last years 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.

The Winterschool is dedicated to molecular nanostructures as a new class of materials. Like the previous winterschools it is supposed to run on an informal level. In addition to the lectures and poster sessions we have arranged a special miniworkshop on "Scientific supplies and industrial needs: The commerzializaiton of carbon nanophases". This workshop takes place on Tuesday, March 7 from 3 pm to 5 pm. It is part of the IWEPNM 2006 program.

This years IWEPNM is an anniversary as it is the 20th event of this type in Kirchberg. On occasion of this anniversary we will have a special celebration on Wednesday night with a laudatio presented by Michael Mehring and a scientific contribution by Sumio Iijima. The lectures will highlight both the development of the special Kirchberg events and the scientific subjects presented there in recent years. All participants including accompanying persons are invited to participate at this session.

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:

Andreas Stangl	(general assistance, receipts, computers)	Martin Hulman	(Miniworkshop)
		Viktor Siegle	(video side room)
Rudi Pfeiffer	(technical assistance, video transfer, poster)	Michael Schmid	(presentations, microphone)
Christian Hölzl	(Miniworkshop, commercials)	Christoph Schaman	(program, poster)

We want, at this point, acknowledge their help for the organization of the IWEPNM 2006. Also, the manager of the Hotel, Frau Mayer, and her staff promised to help us wherever they can.

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

Sincerely yours,

Hans, Peter, Siegmar, Christian

PS: If you want to buy a ticket for the ski lifts in the Kirchberg/Kitzbühel area, ask at the Hotel reception on Saturday evening.
PPS: Internet connection through WLAN is available for all participants, even if they are not accommondated at the Hotel Sonnalp. Please check at the front desk.

INTERNATIONAL WINTERSCHOOL on ELECTRONIC PROPERTIES of NOVEL MATERIALS

MOLECULAR NANOSTRUCTURES

CHAIRMEN: H. KUZMANY (Vienna)
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P. Rudolf (NL)
C. Schönenberger (CH)
R.E. Smalley (†)
C. Thomsen (D)
A. Zettl (US)

SCOPE

This winterschool will provide a platform for reviewing and discussing new developments in the field of electronic properties of molecular nanostructures and their applications. Subjects included are: • carbon nanotubes: mechanical & electronic properties, • fullerenes & fulleroides, • ab initio calculations for molecular nanostructures, • single molecule experiments, • scanning electron microscopy and spectroscopy of molecular nanostructures, • applications of molecular nanostructures, • molecular nanostructure composites, • molecular nanostructure chemistry, • molecular machines and molecular motors, • template grown molecular nanomaterials

INFORMATION FOR PARTICIPANTS

Time and location

The IWEPNM 2006 starts on Saturday, March 4, evening at the HOTEL SONNALP in Kirchberg / Tirol, Austria and extends to Saturday, March 11, breakfast. There will be a reception party on March 4, after dinner and a farewell party including dinner on Friday, March 10.

Transport

The hotel Sonnalp can be reached by privat car from downtown Kirchberg by driving about one kilometer towards Aschau. Participiants 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 2006, 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`
However, all questions concerning the the IWEPNM 2006 should be directed to:
Prof. H. Kuzmany, Institut für Materialphysik, Universität Wien
Strudlhofgasse 4 A–1090 Wien, Austria
Tel: ++43 1 4277 51306, Fax: ++43 1 4277 51375
email: `hans.kuzmany@univie.ac.at`
WWW: `http://www.univie.ac.at/spectroscopy/iwep.htm`

Participation

Participation at the IWEPNM 2006 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 at each lecture. Overhead projections and presentations using data video projection will be possible. Presentation of video films needs prearranged confirmation. Posters will be presented in the hall of the seminar room.

Proceedings

The contributions to the IWEPNM 2006 will be published by physica status solidi. The expected date of appearance of the proceedings is September 2006.

Guidelines for the preparation of the manuscripts can be picked from the web site of the IWEP. A hardcopy is attached to this program booklet. Manuscripts must be submitted by e-mail to Sigmar Roth at `iwep@fkf.mpg.de`.

They can only be published if they arrive before April 20, 2006. 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.

IWEPNM 2006
CHAIRPERSONS FOR THE ORAL SESSIONS

The following participants are asked to support the program of the winterschool by serving as chairperson.

Sun., 05.03.	morning	INTR	Forró
	morning, after coffee break	TRP1	Jarillo-Herero
	evening	TRP2	Bockrath
Mon., 06.03.	morning	PREP	Zakhidov A.
	morning, after coffee break	PREP	Simon
	evening	APPLe	Fischer
Tue., 07.03.	morning	OPTE	Hartschuh
	morning, after coffee break	OPTE	Machon
	miniworkshop	MWS	Hulman
	evening	RSL	Lefrant
Wed., 08.03.	morning	TGNM	Kavan
	morning, after coffee break	TGNM	Rudolf
	evening	NME	Tang Z.
	night	CEL	
Thu., 09.03.	morning	THEO	Kürti
	morning, after coffee break	THEO	Doorn
	evening	APPLc	Baughman
Fr., 10.03.	morning	SME	Obraztsova
	morning, after coffee break	NCNT	Pichler
	evening	APPLb	Hone

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

Chairpersons please remember: **YOU HAVE TO ASK FOR QUESTIONS FROM THE SIDEROOM!**

Chairpersons please remember: **FOR QUESTIONS FROM THE MAIN ROOM PLEASE ASK THE SPEAKER TO REPEAT THE QUESTION. THE MICROPHON 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

IWEPNM2006 - Final program

Final program schedule: morning							
Sess. Day	**08:30**	**09:00**	**09:30**	**Break**	**10:30**	**11:00**	**11:30**
Sat 4.3.							
Sun 5.3. INTR & TRP1	Carbon nanotubes electronics & opto-electronics **AVOURIS, US**		Electronic properties of semiconducting carbon nanotubes **FUHRER, US**	**C**	Four-point resistance of nanotubes **BACHTOLD, E**	High-Tc supercond. d in entirely end-bonded carbon nanotubes **HARUYAMA, J**	Electric transport phenomena in nanotubes and grapheme **KIM, US**
Mon 6.3. PREP	From super growth to DWNT forests, CNT solids, flexible transparent CNT films and ….. **HATA, J**	Towards chirality controlled synthesis of single-walled carbon nanotubes **KONG, US**	Utilizing the inherent redox differences of SWCNTs to ractionalize them … **PAPADIMITRAKOPULOS, US**	**O** **F** **F**	Studies of the role of atomic hydrogen in the growth of SWNT and vert. aligned CNTs	Novel catalysts, RT and the importance of oxygen for the synthesis of SWCNT **RÜMMELI, D**	Fullerene-functionalised carbon nanotubes - novel hybrid nanomaterial **KAUPINNEN, FI**
Tue 7.3. OPTE	Recent advances in the optical spectroscopy of single-walled carbon nanotubes **HEINZ , US**		Excitons & the optical response of nanotubes and nanowires **LOUIE, US**	**E** **E**	Excitons in carbon nanotubes **MAULTZSCH, D**	Magneto-optical spectroscopy of excitons in CNTs **KONO, US**	Exciton dynamics in carbon nanotubes **HERTEL, US**
Wed 8.3. TGNM	HR-TEM imaging of molecules and ions trapped inside carbon nano-spaces **SUENAGA, J**	Struct. correlation of band-gap modific. induced in HgTe by dimens. constraint in.. **SLOAN, UK**	Tube-tube interaction in template grown SWCNTs **PFEIFFER, A**	**B** **R**	NMR evidence for uniform el. prop. in a macroscopic set of DWCNT **ALLOUL, F**	Conduction electron spin resonance of SWCNTs **FORRO, CH**	C59N monomer spins inside single-wall carbon nanotubes: rotational dynamics, CT, & local DOS. **SIMON, HU**
Thu 9.3. THEO	Electron phonon coupling in carbon nanotubes **MACHON, D**	Electron phonon coupling, Raman spectra & el. transport in NTs **FERRARI, UK**	Hot phonons in CNTs and superconductivity in Ca intercalated graphite **MAURI, F**	**E** **A** **K**	Superconductivity in carbon: from C60 to diamond **SAITO, J**	Chirality control of carbon nanotubes by epitaxial growth **REICH, US**	Chirality control of carbon nanotubes by epitaxial growth **CARLSSON, D**
Fri 10.3. SME, NCNT	Three-terminal transport through molecular junctions **V D ZANT, NL**	Measurement of the conductance of single conjugated molecules **YACOBY, IL**	Pair tunneling through single-molecule junctions **VON OPPEN, D**		C-N and C-BN SWNTs: growth and structural properties **LOISEAU, F**	Silicon nanowires as electronic devices: CVD growth & characterisation **DÜSBERG, D**	Ultra-precise molecularly thin semiconductor shells: from nanotubes to nanocorrugated quantum Systems **PRINZ, RU**
Sat **11.3.**	**Departure**						

Final program schedule: afternoon							
12:00	**17:00**	**18:30**	**19:00**	**19:30**	**20:00**	**20:30**	**Sess. Day**
		Reception Party 21:00					**Sat 4.3.**
M **I** **N**	**D** **I** **N**	Quantum Transport in Nanowires and Nanotubes **KOUVENHOVEN,NL**	Aharonov-Bohm effects in multiwall carbon nanotubes **STRUNK, D**	Observation of an oscillating mag. resistance with gate voltage in CNT based TMR devices **SCHÖNENBERGER,CH**	Measurements of thermal conductivitiy of individual carbon nanotubes **FUJII, J**		**Sun 5.3.** TRP2
I W	N E	Near-infrared fluorescence of single-walled carbon nanotubes: applications **WEISMAN, US**	Transport measurements in nanotubes with known (n,m) indices **HONE, US**	Solid-state fabrication, structure, multifunctional appl. of CNT yarns & transp. sheets **BAUGHMAN, US**	Novel mesophase nanocomposite organic photovoltaics **CAROLL, US**	SWCNT polymer composites: properties & implications for practical use **HORNBOSTL, D**	Mon 6.3. APPLe
O R K Scientific supplies and industrial needs: The commer-cialization of carbon nanophases	R	Int. issues & screening of excitons in quasi-1d CNTs & res. profile of 1d carb. chains **JORIO, BR**	Nanoscale spectroscopy with optical antennas **NOVOTNY, US**	Photolum. studies of cross-polarized absorption of SWCNTs **MARUYAMA, J**	**Poster A - L**		Tue 7.3. RSL
S H	18:30	Macroscopic transport by synthetic molecular machines **RUDOLF, NL**	Nano-electromechanical devices based on single-walled carbon nanotubes **MEYER, D**	Rotor-stator phases of fullerees with cubane derivatives : A novel family of ….. **PEKKER, HU**	Break 20:10 Twenty Intern. Winterschools in Kirchberg: How come? **MEHRING, D**	20:50 Nano-carbon materials: formation, characterization, and applications **IIJIMA, J**	Wed 8.3. NME, CEL
O P S		Surface chemistry & heterogeneous catalysis of carbon nanostructures	Chemical functionalization of fullerenes and carbon nanotubes **HIRSCH, D**	Exploiting the intrinsic prop. of SWCNTs for transp. & delivery of biol cargos & trig. cell death **WONG, US**	**Poster M - Z**		Thu 9.3. APPLc
17.00	In vitro evaluation of possible adverse effect of nanosized materials **BRUININK, CH**	DNA-decorated carbon nanotubes for chemical sensing **JOHNSON, US**	Carbon nanotube networks as a material for probing biological interactions **ARTUKOWICH , US**	Summary **PICHLER, D**		Bauernbuffet, farewell	Fri 10.3. APPLb
							Sat 11.3.

PROGRAM

AND

ABSTRACTS

Introduction & Transport I

8:30 – 9:30	**P. AVOURIS, US** *Carbon nanotube electronics and optoelectronics*
9:30 – 10:00	**M.S. FUHRER, US** *Electronic properties of semiconducting carbon nanotubes*
10:00 – 10:30	**Coffee break**
10:30 – 11:00	**A. BACHTOLD, E** *Four-point resistance of nanotubes*
11:00 – 11:30	**J. HARUYAMA, JP** *High-Tc superconductivity in entirely end-bonded carbon nanotubes*
11:30 – 12:00	**P. KIM, US** *Electric transport phenomena in nanotubes and graphene*
12:00 – 17:00	**Mini Workshops**
17:00 – 18:30	**Dinner**

Transport II

18:30 – 19:00	**L.P. KOUVENHOVEN, NL** *Quantum Transport in Nanowires and Nanotubes*
19:00 – 19:30	**C. STRUNK, D** *Aharonov-Bohm effects in multiwall carbon nanotubes*
19:30 – 20:00	**C. SCHÖNENBERGER, CH** *Observation of an oscillating magnetoresistance with gate voltage in carbon-nanotube based TMR devices*
20:00 – 20:30	**M. FUJII, JP** *Measurements of thermal conductivitiy of individual carbon nanotubes*

8:30 INTR 1

Carbon nanotube electronics and optoelectronics

Phaedon Avouris
IBM T.J. Watson Research Center

Carbon nanotubes (CNTs) have properties that make them ideal for applications in both nano- and optoelectronics. Although a variety of different electronic devices based on CNTs have been demonstrated, most of the emphasis has been placed on CNT field-effect transistors (CNTFETs). These devices have in many respects characteristics superior to conventional devices. However, they also pose a set of new challenges. These include understanding the new 1D transport physics, the increased electrical noise, the Schottky barriers at CNT-metal contacts and the ambipolar behavior of vertically-scaled CNTFETs. I will discuss approaches to resolve these problems and produce high performance nanotube devices as well as multi-component single nanotube circuits.

We have used ambipolar (a-) CNTFETs to simultaneously inject electrons and holes with a fraction of these recombining radiatively to produce an electrically-excited, single nanotube molecule light source. Unlike conventional p-n diodes, a-CNTFETs are not doped and there is no fixed p-n interface. Thus, the emitting region can be translated at will along a CNT channel by varying the FET gate voltage. We have found that much stronger localized electroluminescence can be generated at defects or inhomogeneities that introduce potential drops. The emission is the result of intra-molecular impact excitation of electron-hole pairs by the accelerated ("hot") carriers. Localized electroluminescence provides a high brightness IR source and a novel probe of defects, charging, and other otherwise difficult to observe inhomogeneities.

9:30 TRP1 1

Electronic properties of semiconducting carbon nanotubes

Michael S. Fuhrer
Department of Physics and Center for Superconductivity Research, University of Maryland, College Park, MD 20742, USA

The growth of individual, long (> 1 mm), high-quality single- or few-walled carbon nanotubes (CNTs) on substrates by chemical vapor deposition has allowed the careful study of their intrinsic electronic properties. We have studied semiconducting CNTs up to 800 microns in length in a field-effect transistor (FET) geometry, and determined that the charge carrier mobility can be greater than $100,000\,\mathrm{cm}^2/\mathrm{Vs}$ at room temperature, exceeding that of the best known semiconductors. The FET behavior at high bias indicates that semiconducting CNTs do not experience current saturation due to optical phonon emission (as in metallic CNTs) but rather show saturation of the carrier velocity at $\approx 2 \times 10^7$ cm/s, $\approx 3\times$ higher than for Si FETs. Dissipating milliwatt power in CNT FETs in vacuum produces intrinsic, Schottky-barrier transistors with mid-gap alignment of the metal Fermi level, and concomitant low conductance. Exposure to air recovers high conductance p-type behavior, which cannot be explained by change in the contact work function, but is rather due to p-doping of the nanotube, which reduces the Schottky barrier width for holes. Anomalous (1/f) noise measurements on semiconducting CNTs follow Hooge's law, with a Hooge parameter very close to that of conventional semiconductors.

10:30 TRP1 2

Four-Point Resistance of Nanotubes

Adrian Bachtold
ICN - CNM

We have studied the resistance of single-wall carbon nanotubes (SWNT) measured in a four-point configuration with noninvasive voltage electrodes (1). The voltage drop is detected using multiwalled carbon nanotubes while the current is injected through nanofabricated Au electrodes. The resistance at room temperature is shown to be linear with the length as expected for a classical resistor. This changes at cryogenic temperature; the four-point resistance then depends on the resistance at the Au-SWNT interfaces and can even become negative due to quantum-interference effects.

(1) B. Gao, Y.F. Chen, M.S. Fuhrer, D.C. Glattli, A. Bachtold, Phys. Rev. Lett. 95, 196802 (2005).

High-Tc superconductivity in entirely end-bonded carbon nanotubes

11:00 TRP1 3

Junji Haruyama1, I. Takesue1, N. Kobayashi1, S. Chiashi2, Shigeo Maruyama2, T. Sugai3, and H. Shinohara3
Aoyama Gakuin Univ.1, Tokyo Univ.2, Nagoya Univ.3

Can "one-dimensional (1D) conductor" exhibit superconductivity at finite temperatures? This has been a fundamental question in condensed-matter physics for a long time. A carbon nanotube (CNs) can be the best candidate for investigating this question. We report that entirely end-bonded multi-walled CNs (MWNTs) can exhibit superconductivity with a transition temperature (Tc) as high as 12 K, which is approximately 30 times greater than Tc reported for ropes of single-walled CNs. We find that the emergence of this superconductivity is highly sensitive to the junction structures of the Au electrode/MWNTs. This reveals that either 1.only MWNTs with optimal numbers of electrically activated shells or 2. MWNTs with including a very thin SWNT in the core, which are realized by end bonding, can allow superconductivity due to either 1.intershell effects or 2. strong electron-phonon interaction, respectively.

Electric Transport Phenomena in Nanotubes and Graphene

11:30 TRP1 4

Philip Kim
Department of Physics, Columbia University

In this presentation, we will discuss our recent investigation of mesoscopic transport phenomena in carbon nanotubes and graphene, where quantum mechanically enhanced low dimensional effects are predominant. The subjects include, (1) growth/manipulation of ultralong nanotubes and electrical characterization, (2) electrical transport between nanotube-single molecular junction, (3) unusual quantum Hall effect and observation of Berry's phase in mesoscopic graphene.

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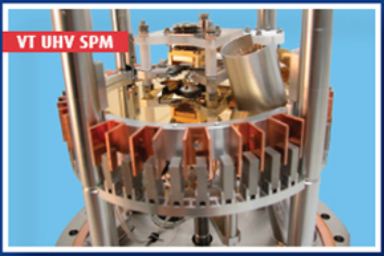

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QUANTUM TRANSPORT IN NANOWIRES AND NANOTUBES

18:30
TRP2 1

Leo P. Kouwenhoven

We study experimentally electron transport in 1 dimensional wires and in particular semiconductor nanowires and carbon nanotubes. The wires and tubes are connected to source-drain contacts with gate electrodes in the substrate or on the surface. In the regime of weak coupling to the contacts we observe standard Coulomb blockade effects. We present level spectroscopy including a determination of the spin states. At proper values of magnetic field and electron number we tune into new Kondo regimes and observe an orbital Kondo effect and orbital+spin, or SU(4)-Kondo effect. In the regime of strong coupling to the contacts interference effects are observed. In this regime and using superconducting contacts, we find supercurrents flowing through InAs-nanowires over micrometer length scales. The critical current is tunable by gate voltage making these devices a realization of the so-called JOFETs (Josephson FETs).

Aharonov-Bohm effects in multiwall carbon nanotubes

19:00
TRP2 2

Christoph Strunk
University of Regensburg

Recent low temperature conductance measurements on multiwall carbon nanotubes in perpendicular and parallel magnetic field are reported. An efficient gating technique allows for a considerable tuning of the nanotube doping level. This enables us to study extensively the signature of nanotube bandstructure in electron quantum interference effects like weak localization, universal conductance fluctuations and the Aharonov-Bohm effect. We show that the weak localization is strongly suppressed at peaks at certain gate voltages which can be linked with the bottoms of one-dimensional electronic subbands. This assignment allows a detailed comparison of theoretical calculations with the experimental data. In agreement with the theory, we find clear indications for a pronounced energy dependence of the elastic mean free with a strong enhancement close to the charge neutrality point. In large parallel magnetic field, we observe a superposition of h/2e-periodic Altshuler-Aronov-Spiva k oscillations and an additional h/e-periodic contribution. The latter contribution shows a diamond-like pattern in the B/Vgate-plane, which reflects the magnetic field dependence of the density of states of the outermost shell of the nanotube.

19:30
TRP2 3

Observation of an oscillating magnetoresistance with gate voltage in carbon-nanotube based TMR devices

Audrey Cottet, Sangeeta Sahoo, Takis Kontos, Jürg Furer, Christian Hoffmann, and Christian Schönenberger
Department of Physics and Astronomy, University of Basel, CH-4056 Basel, Switzerland

One of the basic building blocks of spintronic devices is the spin-valve, which is formed if two ferromagnetic electrodes are separated by a thin tunneling barrier. In such devices, the electrical resistance R depends on the orientation of the magnetization of the electrodes. It is usually larger in the antiparallel than in the parallel configuration. The relative difference of R, the so-called magneto-resistance (MR), is then defined to be positive. The MR may become anomalous (negative), if the transmission probability of electrons through the device is spin or energy dependent. This offers a route to the realization of gate-tunable MR devices, because transmission probabilities can readily be tuned in many devices with an electrical gate signal. Using single and multi-wall carbon nanotubes with ferromagnetic contacts, we demonstrate a spin field-effect. We show that the amplitude and the sign of the MR are tunable with the gate voltage in a predictable manner.

We acknowledge fruitful discussions with R. Egger, C. Bruder and W. Belzig. We thank M. Calame, M. Gräber, S. Ifadir, and D. Keller for the preparation of SWNT devices, C. Sürgers (Karlsruhe) for magnetic measurements, and L. Forro (EPFL) for providing the MWNTs. This work has been supported by the EU RTN network DIENOW, the Swiss National Center (NCCR) on Nano-Scale Science, and the Swiss National Science Foundation.

[1] S. Sahoo et al., Appl. Phys. Lett. 86, 112109 (2005)
[2] S. Sahoo et al. Nature Physics 1, 99 (2005)

20:00
TRP2 4

MEASUREMENTS OF THERMAL CONDUCTIVITY OF INDIVIDUAL CARBON NANOTUBES

Motoo Fujii, Xing Zhang, and Koji Takahashi
Kyushu University, Japan

The paper describes a novel method that can reliably measure the thermal conductivity of a single carbon nanotube(MWCNT) using a suspended sample-attached T-type nanosensor. The experimental results show that the thermal conductivity of a MWCNT at room temperature increases as its diameter decreases, and exceeds 2000 W/mK for a MWCNT with 9.8 nm diameter. The temperature dependence of the thermal conductivity for a MWCNT with 16.1 nm diameter appears to have an asymptote near 320 K.

Preparation

8:30 – 9:00	**K. HATA, JP** *From super growth to DWNT forests, CNT solids, flexible transparent CNT films and super-capacitors and much more*
9:00 – 9:30	**J. KONG, US** *Towards chirality controlled synthesis of single-walled carbon nanotubes*
9:30 – 10:00	**F. PAPADIMITRAKOPOULOS, US** *Utilizing the inherent redox differences of single wall carbon nanotubes to fractionalize them according to diameter and metallicity*
10:00 – 10:30	**Coffee break**
10:30 – 11:00	**R. HAUGE, US** *Studies of the role of atomic hydrogen in the growth of SWNT and vertically aligned carbon nanotubes*
	COMMERCIALS
11:00 – 11:30	**M.H. RÜMMELI, D** *Novel catalysts, room temperature and the importance of oxygen for the synthesis of single wall carbon nanotubes*
11:30 – 12:00	**E.I. KAUPINNEN, SU** *Fullerene-functionalised carbon nanotubes - novel hybrid nanomaterial*
12:00 – 17:00	**Mini Workshops**
17:00 – 18:30	**Dinner**

Application I, electronic

18:30 – 19:00	**R.B. WEISMAN, US** *Near-infrared fluorescence of single-walled carbon nanotubes: applications*
19:00 – 19:30	**J. HONE, US** *Transport measurements in nanotubes with known* (n, m) *indices*
19:30 – 20:00	**R.H. BAUGHMAN, US** *Solid-state fabrication, structure, and multifunctional applications of carbon nanotube yarns and transparent sheets*
20:00 – 20:30	**D.L. CAROLL, US** *Novel mesophase nanocomposite organic photovoltaics*
20:30 – 21:00	**B. HORNBOSTL, D** *Single-walled carbon nanotube polymer composites: properties and implications for practical use*

From Super Growth to DWNT forests, CNT solids, Flexible Transparent CNT films and Super-Capacitors and Much More

8:30
PREP
1

Kanji Hata
Research Center for Advanced Carbon Materials, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8565, Japan

This presentation will provide an overview of our recent development of the "Super Growth" CVD. First, the synthesis of highly efficient impurity free SNWT forest will be described. Second, the growth dynamics will be explored with our recent advance in CNT synthesis. Characterizing of the physical and chemical properties of SWNT forests will be given. Various applications of the super-growth CVD, spanning from material and energy storage to flexible transparent CNT films and super-capacitors would be presented. Third, various new forms of carbon nanotube material, such as DWNT forests and CNT solids, made by utilizing the super-growth technique will be demonstrated. Lastly, challenges and future projects that are planed will be summarized.
[1] K. Hata, D. Futaba, K. Mizuno, T. Namai, M. Yumura, S. Iijima, Science 306 (2004) 1362
[2] Don N. Futaba, Kenji Hata, Takeo Yamada, Kohei Mizuno, Motoo Yumura, and Sumio Iijima, Physical Review Letters,95,056104,(2005)
Corresponding Author Kenji Hata E-mail Tel&Fax , FAX 029-861-4851

TOWARD CHIRALITY CONTROLLED SYNTHESIS OF SINGLE-WALLED CARBON NANOTUBES

9:00
PREP
2

Jing Kong, Hyungbin Son, Stephen Alan Steiner III., Aurea Zare, and Milldred S. Dresselhaus
Electrical Engineering and Computer Science Department, MIT

Single-walled carbon nanotubes are long, thin cylinders of carbon rolled up by a two-dimentional graphene stripe. Due to their unique structures and remarkable properties they are extremely promising for a wide range of applications. Depending on the rolling direction, many possible nanotube structures exist (this is called the chirality of nanotubes, which can be indexed by two integer numbers (n,m)). Different chirality nanotubes have different properties, for example, the chirality of a nanotube determines whether it is semiconducting or metallic, and also determines the size of the semiconductor bandgap. During the past decade tremendous research effort has been devoted to the investigations on nanotube production, properties and applications. Much of the progress has been greatly facilitated by the successful development of synthesizing high yield and high quality nanotube materials. However, none of the synthesis methods so far can produce nanotubes of a specific chirality— which is a critical factor that many applications are relying on. Not only is such knowledge lacking currently, as well as a good understanding on the growth mechanism of carbon nanotubes in the synthesis process. Here at MIT, we are making an effort to tackle such a critical problem. In this talk, I will present our latest progress in this direction.

Utilizing the Inherent Redox Differences of Single Wall Carbon Nanotubes to Fractionate Them According to Diameter and Metallicity

9:30
PREP
3

Fotios Papadimitrakopoulos
Nanomaterials Optoelectronics Laboratory, Department of Chemistry, US

Precise control of single wall carbon nanotubes (SWNTs) over length, diameter, type (or otherwise termed metallicity (metallic vs. semiconducting)) and chirality are of pivotal importance for their future involvement in high-end electronic and optoelectronic devices as well as in biosensory applications. From an electronics perspective, separation of SWNTs according to type and diameter (the latter of which controls the band-gap for semiconducting SWNTs) is of extreme importance. During the past three years a number of separation methodologies have been debuted and although large-scale enrichment remains a challenge, considerable progress have been achieved in this frontier. Our initial report on the preferential interaction of surfactant amines with sem-SWNTs, as opposed to met-SWNT fraction, provided the means to alter their respective solubility characteristics and afford separation.[1] Until recently, very little was known on the underlying nature of this separation. In this contribution, the differential dedoping characteristics of SWNTs according to diameter and metallicity will be described as the fundamental cause that triggers this separation.[2] This was deduced with the help of resonance Raman spectroscopy in conjunction with modeling of the Gibbs free energy and charge-loss as it pertains to the (n,m)-dependent SWNT integrated density of states (IDOS) across a redox jump.
1. D. Chattopadhyay; I. Galeska; F. Papadimitrakopoulos, J. Am. Chem. Soc. 2003, 125(11), 3370-3375.
2. S. N. Kim; Z. Luo; F. Papadimitrakopoulos, Nano Letters, 2005, 5(12), 2500-2504.
Financial support from ARO and AFOSR is kindly appreciated.

10:30 PREP 4

Studies of the Role of Atomic Hydrogen in the Growth of SWNT and Vertically Aligned Carbon Nanotubes

Robert Hauge
Carbon Nanotechnology Laboratory, Rice University, US

The growth of carbon nanotube vertically aligned arrays in the presence of atomic hydrogen has been investigated. Atomic hydrogen was generated with a hot filament in low pressure hydrogen with a few percent of methane. Effects of temperature, pressure, flow rates and methane will be presented. Enriched carbon-13 studies will be discussed with respect to identifying the major reactive carbon species. A description of ongoing efforts to clone preexisting SWNT will also be presented.

11:00 PREP 5

Novel catalysts, room temperature and the importance of oxygen for the synthesis of single wall carbon nanotubes

Mark H. Rümmeli, O. Jost, M. Löffler, R. Schönfelder, A. Grüneis, E. Borowiak-Palen, T. Gemming, T. Pichler, M. Knupfer, M. Kalbác, L. Dunsch, H.-W. Hübers, and B. Büchner
Leibniz Institute for Solid State and Materials Research Dresden, IFW Dresden, P.O. Box 27016 D-64979;01171 Dresden, Germany

Low temperature single wall carbon nanotubes (SWCNT) synthesis is attractive, as it would allow their synthesis to be compatible with microelectronics (below 400-500oC) or biomolecular electronics (100-60oC).
We show that the presence of oxygen, introduced in the form of metal oxides allows metals not normally associated with nanotubes synthesis to become active for the synthesis of SWCNT using laser ablation. Further, the results allow metals with low melting points to be used enabling SWCNT to be synthesized at low temperature (down to room temperature). At these low temperatures their nucleation cannot be explained via fullerene nucleation. We suggest a nucleation mechanism that places a stable oxidized ring as the root cause for the growth of SWCNT.

11:30 PREP 6

Fullerene-Functionalised Carbon Nanotubes - Novel Hybrid Nanomaterial

Esko I. Kauppinen1,3, Albert G. Nasibulin1, Peter V. Pikhitsa2, Hua Jiang3, Paula Queipo1, Anna Moisala1, David P. Brown1, David Gonzalez1, Giulio Lolli4, Arkady V. Krasheninnikov1, Sergey D. Shandakov1, Daniel E. Resasco4, Mansoo Choi2, and David Tománek
1Helsinki University of Technology, Finland, 2Seoul National University, Seoul Korea, 3VTT Processes, Finland, 4University of Oklahoma, USA, 6 Michigan State University, USA

Both fullerenes and single-walled carbon nanotubes (CNTs) are of great interest since they exhibit unique and useful chemical and physical properties. We have discovered a novel hybrid nanomaterial combining these structures, i.e. consisting of fullerenes covalently attached to the outside surface of CNTs, called fullerene-functionalised CNTs. The material structure was investigated by High Resolution Transmission Electron Microscopy (HR-TEM) together with optical spectroscopic and mass-spectrometric techniques. Two one-step continuous i.e. floating catalysts methods for their selective synthesis have been developed: using pre-made iron catalyst particles by a hot wire generator method and particles grown in situ via ferrocene vapour decomposition in the presence of CO and trace amounts of H_2O and CO_2 etching agents. This new material showed a high cold electron field emission efficiency thus making it attractive for many electronic applications, e.g., flat panel displays.

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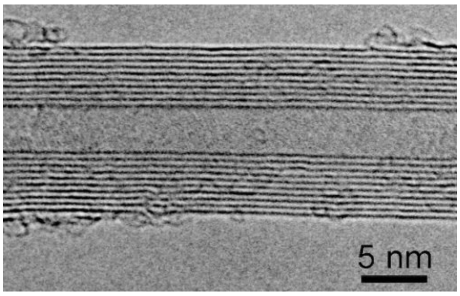
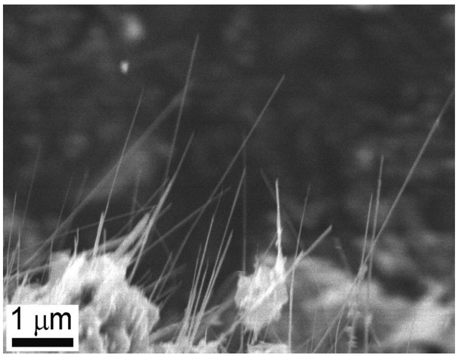
Our MWNTs:

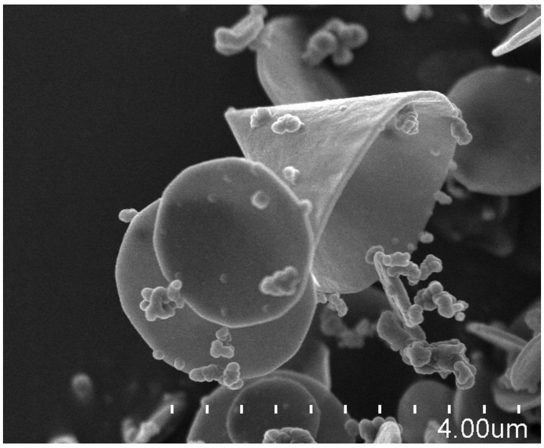
Production method	Arc discharge
Purity	65 wt% carbon nanotubes 35 wt% graphite nanoparticles (impurities)
Diameter distribution	2 - 50 nm
Typical length	> 2 microns (straight tubes)
Chemical composition	100 % carbon no metal particles





Our Carbon Cones and Discs:

Purity	20 wt% carbon cones 70 wt% carbon discs 10 wt% carbon black (impurities)
Size distribution	Wall thickness : 20-50 nm Diameter : 1-3 microns
Chemical composition	C: 98.47 wt% (± 0.50)



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Near-Infrared Fluorescence of Single-walled Carbon Nanotubes: Applications

18:30 APPLe 1

R. Bruce Weisman
Rice University, Houston, Texas, USA

The discovery and spectroscopic assignment of near-infrared photoluminescence from single-walled carbon nanotubes (SWNT) forms the basis for many applications in basic and applied science. Several such applications will be illustrated through current research findings. One important topic is the use of fluorescence spectroscopy for characterizing bulk SWNT samples. Because each (n,m) species of semiconducting SWNT has a known, rather distinct emission wavelength, one can identify the specific species present in a sample from its overall emission spectrum. A turn-key apparatus has been developed that uses this approach to efficiently capture emission spectra and automatically deduce compositional results. Within a period of seconds, spectral data are acquired and analyzed to give relative apparent abundances of specific (n,m) species and nanotube diameter distributions. Another application involves microscopic imaging of SWNT fluorescence. Using a two-dimensional InGaAs array, we have observed emission from individual SWNTs with exposure times in the low millisecond range. Such observations in room temperature aqueous suspensions reveal the translational and rotational diffusion of single nanotubes, as well as thermally-induced bending deformations of longer tubes. The third application area uses near-infrared imaging and spectroscopy to study the interactions of SWNT with biological systems. Because of its high sensitivity and selectivity, this approach allows the tracking of nanotubes in cells, tissues, and organisms. Results will be presented from plant, tissue culture, and animal studies.

Transport measurements in nanotubes with known (n,m) indices

19:00 APPLe 2

James Hone, B. Chandra, R. Caldwell, M. Huang, X.M. Huang, L. Huang, Y. Wang, F. Wang, M. Sfeir, S. O'Brien, T.F. Heinz, and L. Brus
Columbia University

Using a mechanical transfer technique in parallel with efforts to combine optical scattering and structural characteriztion, we have achieved the goal of placing 'the nanotube we want, where we want it.' Long suspended tubes are first grown by CVD and inspected optically. Rayleigh scattering spectroscopy can readily discern between metallic and semiconducting nanotubes, and can be correlated with direct structural probes to provide the exact (n,m) structure. After optical characterization, a chosen nanotube can be transferred to a substrate in the desired location, and devices fabricated using standard e-beam lithography techniques. We have fabricated a number of devices in this manner and are beginning to fully explore the detailed relationship between structure and transport. In addition, we have constructed devices in which the chirality is observed to change along the length of the tube. These devices show electrical transport behavior, including rectification, that is consistent with the chirality changes.

SOLID-STATE FABRICATION, STRUCTURE, AND MULTIFUNCTIONAL APPLICATIONS OF CARBON NANOTUBE YARNS AND TRANSPARENT SHEETS

19:30 APPLe 3

Ray H. Baughman1, M. Zhang1, S. Fang1, A.A. Zakhidov1, M. Kozlov1, S.B. Lee1, A.E. Aliev1, C.D. Williams1, and K.R. Atkinson2
1 University of Texas at Dallas and 2 CSIRO Textile & Fibre Technology, Belmont, Victoria, Australia

We describe novel methods for producing polymer-free carbon nanotube yarns and transparent sheets and describe their properties and applications as multifunctional materials. These fabrication methods start with a solid-state draw to produce a highly oriented aerogel, and involve twist, false-twist, and/or liquid densification processes. The yarns are strong, highly resistant to creep and to knot or abrasion-induced failure and provide a giant tunable Poisson's ratio for stretch in the fiber direction. The nanotube sheets have higher gravimetric strength than the strongest steel sheet or the polymers used for ultralight air vehicles and proposed for solar sails. Applications evaluations are described for artificial muscles, thermal and light harvesting, energy storage, field-emission electron sources, electrically conducting appliqués, three types of lamps and displays, and sensors.

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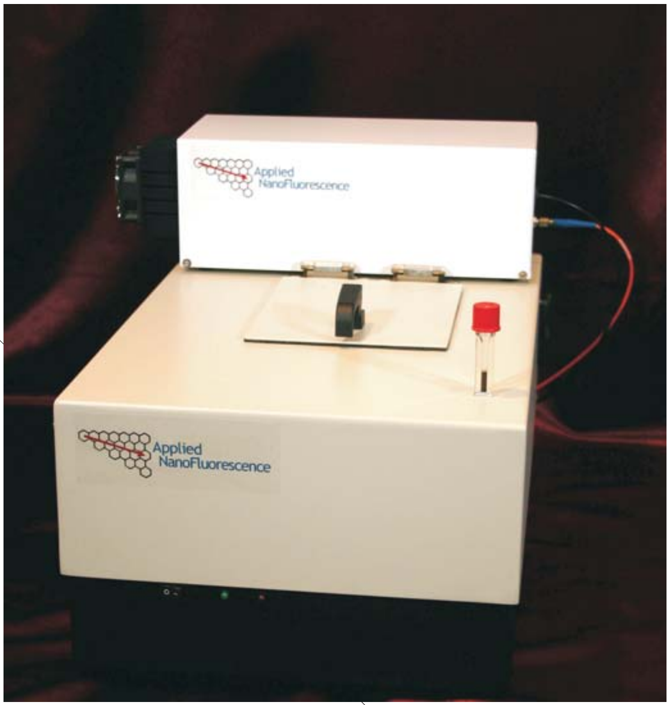

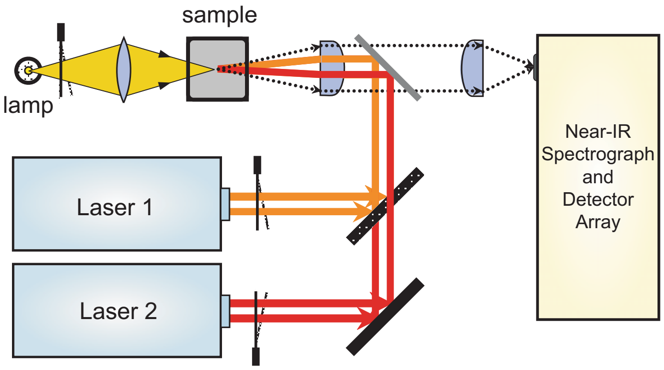

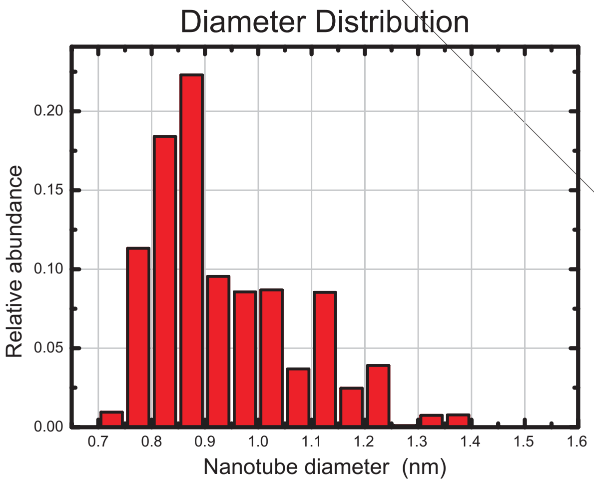

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NOVEL MESOPHASE NANOCOMPOSITE ORGANIC PHOTOVOLTAICS

20:00 APPLe 4

David L. Carroll
Wake Forest University, Department of Physics, Winston-Salem NC 27109

Formation of a controlled fullerene mesophase within an organic host system has enabled us to create high-power conversion efficiency photovoltaics. This mesophase is formed using thermal gradients that provide a fluidic mobility of the fullerenes and allow for the creation of noneqilibrium morphologies in the nanocrystalline 1-(3-methoxycarbonyl)propyl-1-phenyl-(6,6)C61 (PCBM) within regioregular poly(3-hexylthiophene) (P3HT). From this reorganization of the component materials in the matrix the overall efficiency of the system jumps dramatically from the roughly 2.4% to nearly 6%.

Single-walled Carbon Nanotube Polymer Composites: Properties and Implications for Practical Use

20:30 APPLe 5

Björn Hornbostel, and S. Roth
Max Planck Institute for Solid-State Research

This contribution presents a comprehensive evaluation of single-walled carbon nanotubes composites where a polymer matrix was chosen as a host matrix. The regarded aspects involve considerations on electric conductivity, electromagnetic shielding, heat conductivity, dilatometry and the mechanical stability. It is well known that carbon nanotube polymer systems conduct electric current at much lower loads of filler material in comparison to globular fillers like carbon black. But a positve influence of SWCNTs' high tensile loading values on the entire polymer system is debatable. It is shown that the incorporation of single-walled carbon nanotubes can improve the mechanic stability but not self-evidently and strongly dependent on the host system. A new approach to realize a mechanically highly robust polymer composites is presented. These plastics evince a high modulus of elasticity at an early percolation threshold and consist of three components.

Optical excitation

8:30 – 9:30	**T.F. HEINZ, US** *Recent advances in the optical spectroscopy of single-walled carbon nanotubes*
9:30 – 10:00	**S.G. LOUIE, US** *Excitons and the optical response of nanotubes and nanowires*
10:00 – 10:30	**Coffee break**
10:30 – 11:00	**J. MAULTZSCH, D** *Excitons in carbon nanotubes*
	COMMERCIALS
11:00 – 11:30	**J. KONO, US** *Magneto-optical spectroscopy of excitons in carbon nanotubes*
11:30 – 12:00	**T. HERTEL, US** *Exciton dynamics in carbon nanotubes*
12:00 – 17:00	**Mini Workshop on scientific supplies and industrial needs: The commercialization of carbon nanophases:** **ARCS, A, M. HULMAN** *Commercialization of Carbon Nanotubes: On-Market and Near-to-Market Applications* **Nanocyl, B, R. PRADA SILVY** *Nanocyl Carbon Nanotube Industrial Applications* **FutureCarbon, D, W. SCHÜTZ** *FutureCarbon – Carbon Nanomaterials for various applications* **Applied Nanofluorescence, US, B. WEISMAN** *The NanoSpectralyzer: a Turn-Key Instrument for Automatic Analysis of Single-Walled Carbon Nanotube Samples*
17:00 – 18:30	**Dinner**

Raman spectroscopy & luminescence

18:30 – 19:00	**A. JORIO, BR** *Intensity issues and screening of excitons in quasi-onedimensional carbon nanotubes and resonance profile of one-dimensional carbon chains*
19:00 – 19:30	**L. NOVOTNY, US** *Nanoscale spectroscopy with optical antennas*
19:30 – 20:00	**S. MARUYAMA, JP** *Photoluminescence studies of cross-polarized absorption of single-walled carbon nanotubes*

Poster I (A–L)

8:30 OPTE 1

Recent Advances in the Optical Spectroscopy of Single-Walled Carbon Nanotubes

Tony F. Heinz
Columbia University

Optical spectroscopy of single-walled carbon nanotubes (SWTNs) has played a central role in the study of these structures for many years. In this paper, we review some of the exciting recent progress in this field. One of the fundamental issue concerns the physical interpretation of the optical resonances exhibited by all SWNTs: Do these arise from the van Hove singularities in the joint density of states or are they excitonic transitions? Although theory has predicted strong excitonic interactions, until recently there has been neither a clear experimental identification of excitonic features nor a determination of their binding energy. We describe how nonlinear spectroscopy has lead to our current understanding that the transitions are excitonic, with exciton binding energies of 100's of meV.

Another frontier for optical characterization is the characterization of individual SWNTs. Several approaches, including fluorescence, resonant Raman scattering, and Rayleigh (or elastic) light scattering, have been successfully developed. We highlight application of the Rayleigh technique, which permits rapid spectroscopic characterization of both semiconducting and metallic SWNTs. This approach has been applied in conjunction with controlled changes in the local environment, as well as correlated electrical transport and structural analysis of optically characterized individual SWNTs.

9:30 OPTE 2

Excitons and the Optical Response of Nanotubes and Nanowires

Steven G. Louie
Department of Physics, University of California at Berkeley

Owing to their reduced dimensionality, the behavior of quasi-one-dimensional systems is often strongly influenced by electron-electron interaction. We show, through first-principles excited-state calculations, that the optical response of nanotubes and nanowires is qualitatively altered by many-electron interaction effects. It is discovered that exciton states in the semiconducting carbon nanotubes have binding energies that are orders of magnitude larger than bulk semiconductors and hence they dominate the optical spectrum at all temperature, and that bound excitons can exist even in metallic carbon nanotubes. These predictions demonstrate the crucial importance of an exciton picture in interpreting experimental data. In addition to the optically active (bright) exciton states, theory predicts a number of optically inactive or very weak oscillator strength (dark) exciton states. We have performed analysis and modeling of the exciton properties (symmetry, binding energy, exciton size, oscillator strength, and radiative lifetime) as a function of factors such as tube diameter, chirality, temperature, and screening due to external medium. Our studies further show that excitonic effects are equally dominant in the optical response of BN nanotubes and Si nanowires. The physics behind these phenomena is discussed.

10:30 OPTE 3

Excitons in carbon nanotubes

Janina Maultzsch, R. Pomraenke, S. Reich, E. Chang, D. Prezzi, A. Ruini, E. Molinari, M.S. Strano, C. Thomsen, and C. Lienau
Technische Universität Berlin, 10623 Berlin; Max-Born-Institut Berlin, 12489 Berlin; Department of Materials Science and Engineering, MIT, Cambridge, MA 02139-4307; INFM and University of Modena and Reggio Emilia, 41100 Modena, Italy;
University of Illinois, Urbana, IL 61801

We report experimental evidence for large exciton binding in carbon nanotubes [1]. By two-photon luminescence excitation spectroscopy we address exciton states with different wave function symmetry; their separation in energy indicates the magnitude of the exciton binding energy. We determined binding energies of 300-400 meV for nanotubes with diameters between 0.7 and 0.9 nm, almost one fourth of the band gap. We present ab-initio calculations of one- and two-photon absorption, which are in excellent agreement with the experiments. The calculated exciton wave functions are delocalized along the circumference of the tube and extend over several nm along the tube axis. They show the expected symmetry, thus confirming our interpretation of the two-photon experiments.

[1] J. Maultzsch et al., Phys. Rev. B 72, 241402(R) (2005).
[2] F. Wang et al., Science 308, 838 (2005).
[3] E. Chang et al., Phys. Rev. Lett. 92, 196401 (2004).

MAGNETO-OPTICAL SPECTROSCOPY OF EXCITONS IN CARBON NANOTUBES

11:00
OPTE 4

Junichiro Kono
Rice University

This talk will describe our recent optical experiments on single-walled carbon nanotubes in high magnetic fields [1], probing the influence of a tube-threading magnetic flux on their band structure and excited states. The magnetic flux breaks the time-reversal symmetry and thus lifts the K-K' valley degeneracy, and the amount of state splitting is determined by the Aharonov-Bohm phase. We show that this field-induced symmetry breaking overcomes the Coulomb-induced intervalley mixing which is predicted to make the lowest singlet exciton state optically inactive (or "dark") [2]. Each photoluminescence peak, corresponding to a specific chirality, splits into two in a magnetic field, and the magnetic field dependence of the relative intensities of the two peaks reveals that the lower-energy peak increases in intensity (or "brightens") with increasing field. These results can be understood in terms of magnetic brightening of an excitonic state that is dark at 0 T, in agreement with a very recent calculation [3].

1. S. Zaric et al., Science 304, 1129 (2004); Nano Lett. 4, 2219 (2004); Physica E 29, 469 (2005); Phys. Rev. Lett., to appear (see also cond-mat/0509429).
2. H. Zhao and S. Mazumdar, Phys. Rev. Lett. 93, 157402 (2004); V. Perebeinos et al., Nano Lett. 5, 2495 (2005); C. D. Spataru et al., Phys. Rev. Lett. 95, 247402 (2005).
3. T. Ando, J. Phys. Soc. Jpn. 75 (2006), to appear.

EXCITON DYNAMICS IN CARBON NANOTUBES

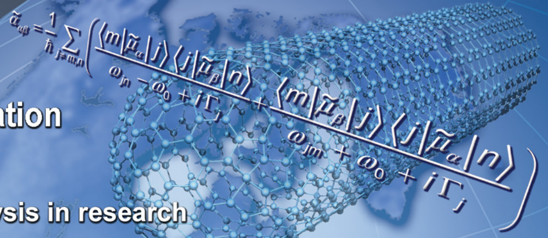
11:30
OPTE 5

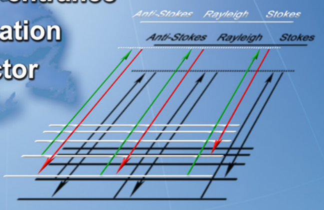
Tobias Hertel, Jared Crochet, and Zipeng Zhu
Vanderbilt University

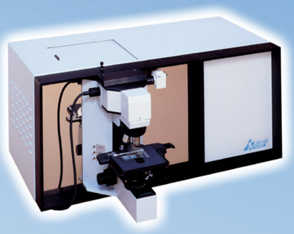
The spectroscopy of excitons in semiconducting single-wall carbon nanotubes and our understanding of their character and dynamics has witnessed tremendous progress over the last 4 years. New synthesis- and post synthesis processing techniques recently advanced, for example by the Resasco group [1] and Arnold et al. [2] were found to be of great benefit for such studies. I discuss how this helps to shed new light onto fundamental processes underlying exciton dynamics, exciton-exciton interactions and their decay. CW photoluminescence, time-resolved pump-probe spectroscopy from the THz to the visible range of the spectrum as well as newly developed pump-probe excitation spectroscopy (PPES) are used for investigation of the coupling of electronic with vibrational degrees of freedom. Moreover I will report on experiments aimed at a better understanding of tube length or tube-tube interactions for E11 and E22 exciton dynamics, exciton delocalization and photoluminescence decay.

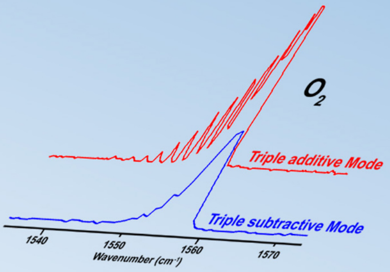
Fruitful collaborations with the Hersam group, the Resasco group, the Strano group, and the Wolf group are gratefully acknowledged.

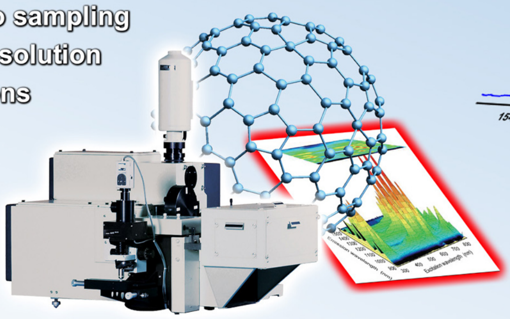
[1] Kitiyanan, B., W.E. Alvarez, J.H. Harwell and D.E. Resasco, Chem. Phys. Lett., 317 (2000) p497.
[2] Arnold, M.S., S.I. Stupp and M.C. Hersam, Nano Lett., 5 (2005) p713.


$$\tilde{\alpha}_{\alpha\beta} = \frac{1}{\hbar}\sum_{j\neq m,n}\left(\frac{\langle m|\tilde{\pi}_\alpha|j\rangle\langle j|\tilde{\pi}_\beta|n\rangle}{\omega_{jn}-\omega_0+i\Gamma_j}+\frac{\langle m|\tilde{\pi}_\beta|j\rangle\langle j|\tilde{\pi}_\alpha|n\rangle}{\omega_{jm}+\omega_0+i\Gamma_j}\right)$$









INTENSITY ISSUES AND SCREENING OF EXCITONS IN QUASI-ONE DIMENSIONAL CARBON NANOTUBES AND RESONANCE PROFILE FOR ONE-DIMENSIONAL CARBON CHAINS

18:30 RSL 1

Ado Jorio, P.A.T. Araujo, L.G. Cancado, C. Fantini, and M.A. Pimenta
Physics Department, Universidade Federal de Minas Gerais (UFMG). Belo Horizonte, BRAZIL

We use resonance Raman spectroscopy to analyze the so-called Kataura plot for the quasi-one dimensional carbon nanotubes, and show evidence for the screening of excitons. We also analyze the (n,m) dependence for the Raman (radial breathing mode) scattering and photoluminescence efficiencies, important for population characterization. Based on this analysis we prove chirality dependence, including the existence of a node in the radial breathing mode intensity for specific (n,m) tubes, as predicted by theory. We also analyze some intensity issues related to the disorder-induced D band, important for defect characterization. Finally, we present the resonance profile and lineshape analysis for a 1850cm-1 Raman feature assigned to strictly one-dimensional carbon chains.

Nanoscale spectroscopy with optical antennas

19:00 RSL 2

Lukas Novotny, P. Anger, N. Anderson, and A. Hartschuh
University of Rochester and University of Tuebingen

Because of diffraction, propagating radiation cannot be localized to dimensions smaller than half the optical wavelength. To overcome this limit, we use optical antennas to localize radiation to length-scales much smaller than the wavelength of light. We place a laser-irradiated optical antenna, such as a bare metal tip, a few nanometers above a sample surface in order to establish a localized optical interaction and a spectroscopic response (fluorescence, absorption, Raman scattering, ..). A high-resolution, hyperspectral image of the sample surface is recorded by raster-scanning the antenna pixel-by-pixel over the sample surface and acquiring a spectrum for each image pixel. We have applied this type of near-field optical spectroscopy to map out the vibrational modes of individual single-walled carbon nanotubes (SWNT) with a resolution of 10nm. The method is able to resolve defects in the tube structure as well as interactions with the local environment. The proximity of the antenna influences the local light-matter interaction and affects the selection rules, the quantum yield, and momentum conservation. To study these effects, we have measured the fluorescence enhancement and quenching of a single molecule as a function its orientation and distance from the antenna.

Photoluminescence studies of cross-polarized absorption of single-walled carbon nanotubes

19:30 RSL 3

Shigeo Maruyama
The University of Tokyo

Though our previous studies of photoluminescence (PL) of single-walled carbon nanotubes (SWNTs) consisting of carbon-13 (SW13CNTs) synthesized from isotopically modified ethanol [1], we have found the excitonic phonon sideband peak due to the strong exciton-phonon interaction with the expected isotope shift [2]. Phonon sideband features observed for (7,5) and (6,5) nanotubes are remarkably similar to the excitonic phonon sideband predicted by Perebeinos et al. [3]. In addition to these phonon sideband features, we also found low-intensity "epure electronic" peaks whose origin has never been discussed. In order to examine these "epure electronic" features, polarized PLE measurements on individually-dispersed SWNTs aligned in a gelatin-based thin film. By comparing optical transitions of SWNTs for incident light parallel or perpendicularly polarized to the nanotube axis, we have attributed these features to excitation by cross-polarized light to the nanotube axis. Finally, the cross-polarized absorption energies and line-shapes are compared with cross-polarized version of the Kataura plot.

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KINETICS OF FULLERENE DISSOLUTION IN NON-POLAR SOLVENT

PTue 1

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Since the discovery of fullerenes in 1985, the study of fullerene solutions has been a point of interest for many researchers due to various interesting properties and promising, e.g. medical, applications. In many different solvents fullerenes tend to form clusters [1]. One of the interesting effects observed in the solutions of C_{60} is the kinetics of fullerene dissolution. Particularly, a decrease in the fullerene concentration in time in the C_{60}/CS_2 solution was revealed in experiments on the light absorption [2] and small-angle neutron scattering [3].

In the present work we develop a theory of fullerene dissolution to explain this effect. The basic kinetic equations, describing cluster formation and growth in fullerene solutions [4], are modified with two additional terms. These terms introduce the flow of single fullerene molecules from the solid phase and the processes of sedimentation of large fullerene clusters from the solution.

The proposed model qualitatively describes the observed behavior of C_{60} concentration in the solutions. Various regimes of the obtained kinetics as a function of model parameters are predicted.

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CVD SYNTHESIS OF CARBON NANOTUBES DEVOTED TO ULSI ELECTRONIC APPLICATIONS

PTue 2

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Since their discovery, Single-Wall Carbon Nanotubes (SWCNTs) have been presented as one of the most promising materials for developing nanoelectronic devices such as Carbon Nanotube Field Effect Transistor (CNT-FET).

While prototypes have demonstrated that is possible to make CNT PMOS devices that compete with the more advanced technologies available and that exhibit a carrier mobility that is twenty times higher than in Si devices, a great effort is still required to develop the necessary technology that may allow CNT integration into ULSI circuits.

To this aim, CVD has been shown to be the most appealing CNT growth technique, but up to now a full control on nanotube in situ growth parameters is lacking.

Pursuing this goal, we report a comparison on the behavior of different catalyst preparations (Fe, Mo, Ni and mixture, obtained from different precursors and processes) while varying thermodynamic conditions and carbon feedstock.

Above all, we have focused our research on the different behaviour of alcohols and hydrocarbon gasses due to the different H/C/O ratio.

PHOTOLUMINESCENCE MAPPING OF LENGTH-SEPARATED SINGLE-WALLED CARBON NANOTUBES

PTue 3

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We will present near-infrared photoluminescence mapping of length-defined individual single-walled carbon nanotubes (SWNT) separated in water-surfactant dispersions by size exclusion chromatography. Furthermore, we investigated the ultrasonic induced scission of different SWNT materials by AFM, Raman and absorption spectroscopy. The influence of different parameters on the scission rate was studied.

PTue 4

THERMAL EFFECTS in RAMAN SPECTRA of HEXAGONAL BORON NITRIDE and NANOTUBE-CONTAINING BORON NITRIDE SOOT

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Single-wall BN nanotubes (BNSWNT) [1] are wide-band semiconductors with ultimate physical properties. A “fingerprint” feature is needed for their unambiguous diagnostics. For carbon SWNT it is a specific Raman spectrum (RS). Unfortunately a unique BNSWNT Raman spectrum has not been observed yet due to the non-efficient purification procedures and a non-resonant BNSWNT RS (in visible). In situ Raman measurements in the growth chamber could help to solve the problem. The process runs at T¿3000C. In this work we have performed the model measurements with a hexagonal BN (h-BN) to be prepared for taking into account the temperature-induced changes in RS of BN SWNT. The nonlinear T-dependence (100–600K) of the tangential Raman mode of h-BN at 1366 cm-1 (in oven) has been obtained. At T¿250 K linear approximation gives 0.01 cm-1/K shift. The oven and laser heating has been compared. Under the laser heating with the same power densities the BNSWNT-containing soot demonstrated much bigger shifts (up to 30 cm-1) than h-BN. A similar difference was observed for HOPG and carbon SWNT.

The work is supported by RFBR-04-02-17618, RAS Presidium Programs and EGIDE.

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PTue 5

Carbon nanotubes reinforced PE and PEEK: fabrication and characterization

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Carbon nanotubes (CNTs) have generated a great deal of interest particularly as fillers in polymer matrix composite materials. These carbon nanofibers are thought to improve the mechanical, electrical and thermal properties of these composites. However, several difficulties related firstly to the dispersion of nanotubes and their compatibility with the matrix and secondarily to the nature of the binding, need to be resolved prior to practical applications.

In this work, two main approaches are considered for fabricating polyethylene (PE)-CNTs and polyetheretherketone (PEEK)-CNTs composites. In the first case, used as reference, CNTs have been embedded in Polymer matrix without any surface modifications, which consist of non covalent attachment of nanotubes and the polymer.

In order to obtain a covalent linking between nanotubes and the matrix, an other approach has been tested. It’s based on the use of both chemically modified CNTs and polymer.The attachment of functionalized CNTs and Polymer can be possible by using di-functional molecules.

The nature of the binding between CNT and polymer chains has been studied using FT-IR, TEM, SEM and AFM. Furthermore, mechanical and electrical tests have been carried out in order to evaluate if the properties of the polymer were improved by the CNTs addition.

PTue 6

STUDY ON HYDROGEN UPTAKE BY DOPED SINGLE-WALL CARBON NANOTUBES

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We present a study on synthesis hydrogen uptake of boron doped single-wall carbon nanotubes (B-SWCNT). The morphology, chemical composition and crystal structure of the produced samples have been characterized by transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDX) and X-ray diffraction (XRD). The specific surface and porosity of pristine and modified SWCNT have been studied as well.

The functionalized SWCNT were used as a hydrogen-storage material. The hydrogen uptake has been examined with use of following methods:

- Temperature programmed desorption (TPD) at ambient pressure,
- Volumetric method at elevated pressure,
- Thermogravimetric analysis (TGA).

LOCALISATION OF INSERTED SPECIES INSIDE SWNT BUNDLES: EXPERIMENTAL AND AB INITIO STUDY

PTue 7

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The aim of this work is to propose a model of inserted species organisation inside single walled carbon nanotube bundles.

First of all, we present X-rays and neutrons diffraction results obtained on iodine inserted carbon nanotubes (p-doping) [1]. Raman experiments indicate the presence of iodine chains and existence of charge transfer between iodine and carbon nanotubes [1,2]. Diffraction patterns obtained by X-rays and neutrons on the same sample are different and seem contradictory. However this apparent contradiction can be explained using a convenient model for the simulation of the diffraction diagrams, allowing us to conclude on the presence of iodine inside tubes.

This fact shows the necessity of theoretical studies to give a coherent interpretation for all results concerning the localisation of doping species.

The same approach has been used for rubidium inserted carbon nanotubes (n-doping). The results of X-rays and neutrons diffraction experiments are surprising and will be discussed in connection with the question of the expansion or not of the hexagonal tubes framework under insertion and also with the question of the localisation of the rubidium inside this framework. The experimental results will be compared to simulations and combined with ab initio calculations [3].

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MAGNETISM IN FULLERIDES AND AMORPHOUS CARBON

PTue 8

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To determine the origin of the different magnetic properties of TDAE-C_{60}, TDAE-C_{70} and amorphous carbon we have made a comparative study of these systems with C13 NMR, X-band EPR,ferromagnetic resonance and squid measurements. The results show that ferromagnetism in TDAE-C_{60} is connected with a Jahn-Teller distortion of the C_{60} ions and the resulting re-distribution of the unpaired electron spin-density which allows for ferromagnetic coupling and a very small magnetic anisotropy. The TDAE ions are involved in super exchange making the structure three dimensional. The different structural and electronic properties of TDAE-C_{70} prevent ferromagnetic ordering. The hysteresis loop and ferromagnetic like properties of amorphous carbon are on the other hand connected with dangling bonds and large paramagnetic clusters. It seems that these conclusions can be extended to carbon foams.

THERMAL AND ELECTRICAL TRANSPORT IN CARBON NANOTUBES

PTue 9

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We have explored thermal conductivity in nanotubes by heating freestanding nanotube devices with an electrical current and measuring the power required to reach breakdown temperature in the center of the nanotube. We find for nanotube devices shorter than 500 nm the power follows a universal scaling law in the tube radius, providing evidence for ballistic phonon propagation in nanotube devices. We obtain an estimate for the thermal conductance quantum that is in good agreement to theory. Our results demonstrate the unique potential of carbon nanotubes as nanoscale phonon channels.

We are also developing nanomechanical switch devices using multi-walled nanotubes (MWNTs) that exploit the ability of concentric nanotube shells to act as low-friction linear bearings. We electrostatically telescope shells of MWNTs to establish electrical contact and turn the device to a conducting ”on” state. Our data yields an estimate of the retraction force on the inner nanotube shells from the outer shells, in agreement with the theoretically expected value. Our devices can be turned ”off” again by applying a sufficiently large gate voltage to bend the nanotube segments until the connection is broken. We estimate our devices are capable of sub-nanosecond switching times, making them suitable as high-speed memory elements.

PTue 10

SYNTHESIS AND CHARACTERISATION OF IRON FILLED SINGLEWALL CARBON NANOTUBES

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In our study we use a highly efficient and simple methodology based on wet chemistry to fill single-wall carbon nanotubes (SWCNTs) with iron and thus create quantum wires in a bulk. The research shown is unique in that it is the first experimental single-wall carbon nanotubes that have iron continuously within their core for extended length scale. The resulting Fe-filled SWCNTs show ferromagnetic behavior even at room temperature, despite the very small diameter. The intercalation of metals within singlewall carbon nanotube structures is a significant step towards the realization of the potential applications using these materials.

PTue 11

Structural Study of C_{60} and C_{70} Cubane

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Fullerenes and cubane form new high-symmetry heteromolecular crystals. C_{60}-cubane and C_{70}-cubane are the first members of this family [1]. We present the results of a detailed structural study in a wide temperature range, from 100 K to 470 K. We found that the structure of these compounds can be understood from the generic fcc C_{60} lattice. In the highest symmetry case freely rotating fullerenes occupy the fcc lattice sites, and cubanes fill the octahedral voids. We found various phase transitions lowering the temperatures. As expected the free rotation of fullerenes becomes hindered and orientational ordering appears. The orientational transition temperature is exceptionally low, which can be explained by combination of the high symmetry environment of fullerenes, the perfect match of convex fullerene and concave cubane molecular surfaces and the significantly expanded fullerene lattice. The high temperature behaviour of these compounds is also special. Near 470 K the cubane molecules disintegrate but the structure survives; a new fullerene copolymer forms, which is stable up to very high temperatures.

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PTue 12

Simulation of exciton distribution in bilayer organic solar cells

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The locally resolved photogeneration of excitons in bilayer organic solar cells (OSC) was simulated by a detailed optical model. A layering scheme involving up to six different ultrathin films on the substrate was taken into account, including the optical constants, interference effects and resulting standing waves. Thus a strong dependency of local exciton generation on the specific geometry and the wavelength was shown.

To determine the distribution of the generated excitons the continuity equation was solved. By defining the quenching properties of cell interfaces the influence of interface exciton recombination was demonstrated. With given exciton diffusion lengths the generation of charge carriers and the quantum efficiency of Phthalocyanine-C_{60} OSCs was calculated. The applicability of the model is discussed by comparison with experimental data.

The effect of molecular oxygen on the thermal conductance of multi-walled nanotubes – a preliminary investigation

PTue 13

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Whilst the effect of oxygen adsorption on the electrical properties of carbon nanotubes has been investigated extensively, little is known about how oxygen changes the thermal properties of nanotubes.
Here we present a preliminary investigation on the effect of molecular oxygen on the electrical and thermal conductance of multi-walled nanotubes measured simultaneously.
The nanotubes were placed in a vacuum chamber (pressures $< 1 \times 10^{-5}$ mbar) for a prolonged period of time (> 7 days) and continuously heated above 100°C to ensure oxygen desorption. Then pure oxygen was introduced in the chamber using a needle valve (the pressure in the chamber was always $< 3 \times 10^{-4}$ mbar) and the heating of the nanotube was stopped to allow oxygen adsorption.
Thermal and electrical conductance measurements were taken simultaneously on the nanotubes when degassed and in the presence of oxygen. The thermal conductance of the nanotubes increased by a maximum of about 20% upon addition of oxygen. The percentage increase was initially linearly dependent on the amount of oxygen added then at oxygen pressures $> 1 \times 10^{-4}$ mbar saturation of the effect was observed.
The reasons for these changes are proposed to be: i) oxygen adsorption caused a change in the nanotubes phonon modes; ii) the presence of oxygen molecules facilitated the inter-shell transfer of heat in the nanotube.

Synthesis, Isolation and Characterization of New Endohedral Fullerenes M@C$_{72}$ (M = Eu, Sr, Yb)

PTue 14

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We report on new europium, strontium and ytterbium endohedral fullerene cages of the type Eu@C$_{72}$, Sr@C$_{72}$ and Yb@C$_{72}$. Single isomers of Eu@C$_{72}$-I, Sr@C$_{72}$-I, Sr@C$_{72}$-II and Yb@C$_{72}$-I were isolated by multi-step HPLC for the first time. Details of their synthesis, separation and characterization by LDI-TOF mass spectrometry and UV-vis will be discussed. Additionally, EPR spectroscopy of Eu@C$_{72}$-I was performed. A second isomer of europium and ytterbium endohedral C$_{72}$, Eu@C$_{72}$-II and Yb@C$_{72}$-II, has been separated by HPLC and identifed by LDI-TOF mass spectrometry.

Bromination of double-wall carbon nanotubes

PTue 15

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Double-wall carbon nanotubes (DWNTs), synthesized by chemical vapor deposition of methane over Mg1-xCoxO solid solution with small addition of molybdenum, have been brominated using a vapour bromine. Transmission electron microscopy showed the brominated product contains tubular structures and agglomerates of thin graphitic layers, which are likely to appear in the result of carbon nanotubes destruction. Raman spectroscopy detected strong decrease of intensity of the radial breathing modes corresponding to the outer sells of DWNTs. Optical absorption spectrum of the brominated material exhibited features indicating that some carbon nanotubes attached no or small amount of bromine atoms. Annealing of the brominated DWNTs at 100°C resulted in a manifestation of fine structure of the spectrum suggesting detaching of bromine atoms from the tube surface with heating.

PTue 16

FUNCTIONALIZATION OF CARBON NANOTUBES FOR ELECTRONIC AND PHOTOVOLTAIC APPLICATIONS

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Nanometer-scale structures are under heavy investigation for producing innovative materials, composites, and electronic devices of greatly reduced size. Carbon nanotubes in particular are fascinating new nanostructures with exceptional properties However, processing and applications of CNTs are still limited because of the difficulties of manipulation and the low solubility of this material.

To improve their solubility and decrease CNTs aggregation, we explored two general strategies: 1) the covalent functionalization of sp2 carbons of the sidewall with organic groups and 2) the non-covalent functionalization through p-p interactions which allows the formation of stable suspensions, while leaving the graphene structure intact. Both approaches have been used to build new carbon nanotubes based devices for electronic/photovoltaic applications.

The last development led us to synthesize dendrimers directly on the nanotubes and that for several reasons: 1) attachment of dendrimers on CNTs permits to amplify the number of functional groups available for further derivatization without disrupting the p-conjugated system of the nanotubes. 2) Complete hiding of nanotubes under a cloud of saturated functional groups could lead to the creation of molecular wires with their insulating layers. 3) Fine tuning of the dendrimer synthesis could permit to obtain nanotubes with tailor-made properties.

PTue 17

IN SITU OPTICAL ANALYSIS OF THE GAS PHASE DURING THE FORMATION OF SINGLE-WALLED NANOTUBES (C AND BN)

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A reactor developed at ONERA to produce SWCNTs by continuous vaporisation of C:Co:Ni target in a gas flow. Optical diagnostics of the gas plume have been performed using Laser Induced Fluorescence (LIF) and Laser Induced Incandescence (LII) to probe respectively atomic/molecular species (Ni, Co, C2, C3) and soot. LIF measurements reveal a plateau of metal vapour, originating from supersaturated vapour above liquid nanoparticles under our supercooling conditions. The vapour density is seen to drop at about 7 mm above the target as a result of complete solidification of metal-carbon particles. The size evolution of the soot changes from linear to non linear respectively with no metal catalyst and when metal catalysts are present into the flow. The soot size suddenly increases at the same location where catalyst vapours disappear. In situ measurements are showing the influence of liquid nanoparticles on the condensation of carbon and confirming the sketches expected from the V- L-S model.

In the same reactor, boron nitride nanotubes are produced from vaporization of hBN target. Atomic boron vapour is probed by LIF. Its spatial evolution is compared to the temperature profile measured by CARS. The solid products are seen to produce a UV photoluminescence induced by our probe laser.

PTue 18

Functionalization of Carbon Nanotubes: Direct Proof of Sidewall Thioation

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We have used Transmission Electron Microscopy (TEM) to observe the structural changes that have occurred to multi-walled carbon nanotubes (MWCNTs) due to acid-treatment. Following the thioation reaction of the acid-treated MWCNTs using P4S10 in refluxing toluene, we have also used Electron Energy Loss Spectroscopy (EELS) to characterize the changes on the nanotubes due to sidewall functionalization. We have determined that the sulfur content bonded to the nanotubes is significant (0.6 %) in terms of the atomic content of the samples. Raman spectroscopy was used to examine the vibrational changes that occurred to the nanotubes as well as identifying new vibrational modes around 500 cm-1 which confirms creation of characteristic carbon-sulfur bonds.

Magnetic Properties of Carbon Nanofoam

PTue 19

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Ferromagnetism is typically the property of transition metals where there are unpaired electrons in unfilled atomic shells even in the solid. Nevertheless various form of carbon show ferromagnetic or ferromagnetic-like behaviour such as the purely organic ferromagnet TDAE-C$_{60}$, polymerized C$_{60}$ forms, hydrogenated amorphous carbon and cluster assembled carbon nanofoam. This system which has an ultra-low density (2-10 mg/cm3) is obtained by laser ablation of glassy carbon in an argon atmosphere. In carbon nanofoam a large difference between field cooled (FC) and zero field cooled (ZFC) magnetic susceptibility has been observed. Some samples show a maximum in the magnetic susceptibility between 50 K and 100 K characteristic of spin-glasses. A weak ferromagnetic like hysteresis curve has been observed at 2 K between 5 T and 5 T with a saturation magnetization of MS 0.3 emu/g. Proton NMR measurements on absorbed water at room temperature showed the existence of two components in the magnetization decay. One has a T1 of about 0.8 msec and the other of about 200 msec. This demonstrates the inhomogeneous nature of the magnetization in carbon nanofoam with magnetic island embedded in a non-magnetic medium. Similar results are also obtained by EPR where three different well separated magnetic centers with different T1 values have been observed.

TEMPERATURE DEPENDENCE OF RESONANCE RAMAN OF SINGLE-WALLED CARBON NANOTUBES

PTue 20

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Raman scattering from single-walled carbon nanotube (SWNT) samples at various temperatures ($4 - 1000\,\mathrm{K}$) in vacuum are measured. The G-band peak exhibited temperature dependence in Raman shift, peak width and intensity. Especially, Raman shift of the G+ peak showed universal temperature dependence, for the various SWNT samples and for excitation lasers with 3 wavelengths (488.0, 514.5 and 632.8 nm).

On the other hand, some of radial breathing mode (RBM) peaks showed anonymous temperature dependence. With increasing temperature, Raman shift of all RBM peak downshifted and the peak width increased. The intensity of most RBM peaks uniformly decreased with increasing temperature, while that of some RBM peaks increased. The intensity of the RBM peaks that increased with increasing temperature was very small at the room temperature and these peaks could not be observed at all from SWNTs dispersed in solution.

These anonymous RBM features are explained by the transitions by cross-polarized excitation. This enhancement of resonance of cross-polarized absorption at higher temperatures will be discussed in term of the change of the electronic density of states.

Superdense, superstrong SiC nanotubules

PTue 21

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The rocksalt phase of silicon carbide (SiC) is observed only at very high pressures. In fact, zincblende or hexagonal SiC transforms to rocksalt above 100 GPa, while the reverse transformation is always observed below 35 GPa. Despite the numerous and careful theoretical works, the actual driving force as well as the large pressure hysteresis accompanying the reversible transformation are still unexplained. At variance with all the previous studies, here we use a low-pressure, low-temperature technique to synthesize nanotubules of rocksalt SiC in massive amounts that, moreover, remain stable at ambient conditions. By accurate density-functional calculations we find metallization of the bulk rocksalt structure at 35 GPa by band overlap at the X edge of the Brillouin zone, and softening of zone-edge phonons at about 2 GPa, as the candidate mechanisms driving the phase transformation. Apparently, in our nanotubules direct nucleation of rocksalt SiC occurs, in grains growing up to 2 nanometre size. Grain boundary curvature-induced pressure may quench the phonon instability in such nanocrystals down to the lower threshold (2 GPa), below which the onset of mechanical instability forbids further growth by dissolution or fragmentation of the nanograins, thereby preserving the observed rocksalt structure. This is a remarkable example of a material whose unstable, high-pressure phase can be stabilized at ambient conditions upon reducing the grain size in the nanometre range. Superdense SiC nanofibers, with superior elastic moduli and possibly better mechanical properties than ordinary SiC, could have many relevant technological applications.

PTue 22

Preparation and EPR characterization of N@C_{60}- and N@C_{70}-based Peapods

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Endohedral fullerenes like N@C_{60} and N@C_{70} can be used as spin probes for the investigation of single wall carbon nanotubes (SWNT). Using nitrogen-based endofullerenes, peapods can only be prepared using a liquid phase filling procedure, which was optimized with respect to filling efficiency. By invoking spin counting by EPR, it is possible to determine the bulk filling factor reliably.

Continuous-wave (c.w.) EPR measurements were performed using different concentrations of the endohedral nitrogen spin probe. Pulsed EPR was additionally used to determine spin relaxation rates as function of temperature to investigate localization dynamics within the tubes or to check for interaction with itinerant electrons.

Using SWNT grown on silica substrates by CVD, the dominant influence of tube diameter on the inhomogeneous line width of the EPR signals could be demonstrated for the first time. Significant differences in fullerene dynamics between narrow and large diameter peapods are revealed by temperature dependent pulsed EPR experiments. These differences are discussed and can be correlated to the varying interaction between the fullerenes and the nanotube wall.

PTue 23

Structural and electronic properties of Ptn (n=1,3,4,7,13) clusters on single wall carbon nanotube

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A first-principle study of the interaction between metal clusters and single wall carbon nanotube was carried out within Density Functional Theory. The structural and electronic properties of Pt clusters on carbon nanotube $(5, 5)$ are investigated and showing a drastic change in electronic structure of metal cluster and a cross-section-deformation of nanotube placed on metal cluster. Catalyst of Pt clusters on nanotube is also investigated.

PTue 24

Transport in multiwall carbon nanotubes and semiconductor nanowires

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In this work we present a comparative study of electronic transport of two types of mesoscopic samples: multiwall carbon nanotubes and semiconductor nanowires.

We studied a wide range of samples (around 100) with different lengths, contact materials and diameters. In all cases we observed a scaling law of the resistance with temperature and DC voltage. The observed behavior can be understood in terms of the Dynamical Coulomb blockade theory, providing that a single tunnel barrier is present. This hypothetical tunnel barrier would have a resistance of the order of 4000 Ohm and a typical energy of about 40 meV for ALL samples independently of changed parameters. Magnetoresistive study allowed us to correlate the scaling exponent to disorder.

Moreover, we present very low temperature measurements until 50mK. We observed a change of transport regime at low temperatures, the samples following an activated transport regime as a function of the temperature bellow 1K. When we apply a DC voltage in this insulting state, these samples keep their isulator nature until a critical DC voltage, at which they change very abruptly of state, becoming metallic. The 4 samples studied made us able to study the correlation between differents phenomenological parameters, enligthing the role played by disorder in each different regime.

13C NMR CHARACERISATION OF FOUR ISOMERS OF C_{70}-O

PTue 25

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C_{70} had D5d point group symmetry with 5 different types of carbon atom environment and 8 different types of bonds. C_{70}-O can either be formed as epoxides or annulenes. The NMR spectra are inconsistent with annulene formation. Thus, forming C_{70}-O by epoxy-bridging can theoretically result in 8 isomers.
The 8 possible isomers of C_{70}-O can be divided into two classes, with 4 isomers in each. One class has the oxygen atom bridging a 6:6 bond, and corresponds to 1,2-, 5,6-, 19,20-, and 20,21-epoxy[70]fullerene. The other class has the oxygen bridging a 6:5 bond, and correspond to 2,3-, 4,5-, 6,7- and 7,8-epoxy[70]fullerene. We will present a paper on the production, complete purification, and characterisation by 13C NMR spectroscopy of 4 isomers of C_{70}-O. The NMR spectra reveal that all four isomers presented here are in the former class (6:6 bond bridging). There is no evidence for any other isomers in the HPLC chromatogram, we therefore conclude there are no 6:5 bridging epoxides.
It is probably no coincidence that 6:6 bonds are shorter than 6:5 bonds (giving greater local curvature) and that all 4 known isomers of C_{70}-O are 6:6 bridging. A discussion of the preference for the 6:6 bridging will also be presented.
Two isomers (1,2 and 5,6) have been reported before: by Roger Taylor (Sussex) and by Saunders (Yale) through 13C and 3He NMR of mixtures. We confirm these as the two dominant isomers, but also present two new isomers, completing the family of 6:6 bridging epoxides. Furthermore, our spectra are on isomer-pure samples, enabling accurate line assignments to the 4 isomers.

Conducting and transparent SWNT/polymer composites

PTue 26

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Transparent, electrically conductive layers based on indium-tin-oxides (ITO) are currently used for electrode applications. Unfortunately the ITO layers are brittle and cannot be deposit on flexible substrate such like plastics. Additional difficulty lies in the preparation of the thin ITO films which requires a vacuum sputtering technique. An alternative to ITO is offered by the transparent polymer matrix filled with single wall carbon nanotubes. This contributions shows flexible, transparent and conducting poly(methyl methacrylate) (PMMA) composites films prepared using SOCl2 functionalized SWNTs. Optical absorption spectra measured on composite films confirm that the composite preparation procedure conserve the electronic properties (position of the Fermi level) of the p-doped nanotubes in polymer matrix. Due to the doping effect of SOCl2 the electrical conductivity of the composites is improved by factor of 5. The light transmission of the composite films depends on the film thickness and the nanotube concentration. For the films of about $20\,\mu$m thick the transmission between 92 % for 0.1 wt % SWNT content and 46 % for 0.5 wt % of SWNT is measured at 500 nm wavelength. The conductivity of the thin films measured by the four point method is 3.5×10^{-3} S/cm and 4.7×10^{-10},S/cm, respectively.

A DFT STUDY OF CHROMIUM-GRAPHITE INTERACTION

PTue 27

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In recent years, various nanoelectromechanical devices have been built which incorporate an individual carbon nanotube as their key component, either multi-walled [1-3] or - most recently - single-walled [4]. When fabricating all of these devices, first chromium then gold are thermally evaporated onto the CNT. This technique seems to be invariably applied for manufacturing metal pads strongly anchored to carbon nanotubes. In spite of its practical success - or, possibly, just because of it - the detailed mechanisms of the interaction of Cr atoms with the C lattice structure stay largely unexplored.
Here we present the first results of a plane-wave, DFT-based study of the energy landscape of a 2D-periodic cell comprising one or two graphite planes plus a Cr atom or dimer. By using both soft, norm-conserving, or ultrasoft pseudopotentials in the gradient-corrected approximation, we calculated the formation energies and migration barriers for several Cr configurations on both the perfect and defective carbon surface. For the Cr atom we find several stable (chemisorbed) states, both on the perfect surface and at a vacancy. For the Cr dimer, we find evidence of reactive dissociation when approaching a vacancy site, while the same appears to be stably bound to a Stone-Wales defect.

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PTue 28

Metal Oxide Nanoparticles for Improved Electrochromic and Lithium Ion Battery Technologies

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Hot-wire chemical vapor deposition (HWCVD) has been employed as an economically scalable method for the deposition of crystalline tungsten oxide nanorods and nanoparticles. Under optimal synthesis conditions, only crystalline nanostructures with a smallest dimension of ≈ 10–50 nm are observed with extensive transmission electron microscopy (TEM) analyses. The incorporation of these particles into porous films led to profound advancement in state-of-the-art electrochromic (EC) technologies. HWCVD has also been employed to produce crystalline molybdenum oxide nano- rods, particles and tubes at high density. TEM analyses show that the smallest dimension of these nanostructures is ≈ 5–30,nm. Raman analyses and small spot electron diffraction reveal that the materials are highly crystalline and consist of alpha-phase MoO_3. It is possible to fabricate large area porous films containing these MoO_3 nanostructures. Furthermore, these films have been tested as the negative electrode in lithium-ion batteries, and a surprisingly high and reversible capacity ranging from ≈ 650, 1000 and up to 1200 mAh/g has been observed for several different films comprised of crystalline MoO_3 nanoparticles with slightly different morphologies. The synthesis of these novel nanostructured materials and their potential for improving both EC and battery technologies will be discussed at length.

PTue 29

RAMAN STUDIES OF EXCITON-PHONON COUPLING IN SINGLE WALLED CARBON NANOTUBES

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Significant chirality-dependent effects on nanotube Raman intensities have recently been observed whose origins lie in the chirality dependence of exciton-phonon coupling. We present resonance Raman excitation data that demonstrates this dependence in radial breathing mode (RBM) intensities for both E11 and E22 excitation. For E22 excitation, intensities for (n-m)mod 3 = -1 chiralities are significantly more intense than for (n-m)mod 3 = +1, with behavior reversing in E11 excitation. We discuss the results in terms of a new theoretical analysis of exciton-phonon coupling that accurately describes the observations with simple intuitive analytical expressions. Relative intensites can be easily predicted using a newly introduced parameter that is also able to explain a number of anomalies in the observations. We also present the first direct comparison of E11 vs. E22 intensities for a number of chiralities, from which a measure of the relative density of decay pathways for each transition can be attained. Finally, results from the analysis of RBM overtone intensities to directly quantify the magnitude of exciton-phonon coupling elements for several chiralities will be discussed. These studies will be discussed in terms of their consequences for other nanotube optical phenomena, sample characterization, and chirality assignment.

PTue 30

Transport properties of Mo6S3I6 nanowire networks

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We present measurements of resistivity on Mo6S3I6 nanowire networks under different conditions. The room-temperature values of conductivity of as-grown nanowire networks are on the order of 0.04 S/m (at 300K) and show linear I-V characteristics, indicating that - in agreement with band structure calculations - there is a finite density of states at the Fermi level. The conductivity of pristine samples is thermally activated, closely following three-dimensional variable range hopping (VRH) behaviour, where the power B over Exp(-T0/T) equals 1/4. Removal of interstitial iodine from the network by annealing in vacuum gives rise to a cross-over to one-dimensional VRH with B = 1/2 and a concurrent increase in room-temperature conductivity. The introduction of water vapour leads to an decrease in conductivity and reveals that the resistivity of the network is sensitive to interstitial water molecules.

NANOSTRUCTURING CARBON NANOTUBES BY UNCONVENTIONAL SOFT LITHOGRAPHIES

PTue 31

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Carbon Nanotubes (CNT) have been widely studied for their unique electronic properties [1] that motivate research for fundamental and applicative researches. Their high electrical mobility and capacity to support large current density make them valuable as semiconductors and as interconnections in nanoscale circuit. One of the major drawbacks is the difficulty on controlling positioning and alignment of CNTs over a wide area and in a reproducible manner.

We propose the fabrication at submicron resolution of a patterned thin film of CNT by Lithographically controlled wetting (LCW) [2] and Micromolding in capillaries (MIMIC) [3].

The proposed methods allow the patterning CNT dispersion with nanometer-sized structures in short times (few seconds) and in a single step. The processes, which we have demonstrated at submicron and nanometer resolution, are able to promote self-organization in a confined space delimited by the mold features.

We systematically investigated the influence of the concentration of CNT, surfactant and the role of the substrates by AFM.

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SHAPE-SELECTIVE SYNTHESIS OF POLAR SEMICONDUCTOR NANOWIRES

PTue 32

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Polar II-VI semiconductors can nucleate in complex shapes ranging from nanowires to nanoribbons, nanosaws and multipods [1-2]. The full potential of these nanostructures can be realized if they are directly grown into devices. Here we demonstrate the deterministic and fully reproducible shape-selective growth of several morphologies of CdSe and ZnTe nanocrystals by a steady-state vapour transport process [3]. The key step in order to achieve reproducible shape selectivity for a given set of deposition parameters is to exclude any effects of temperature ramping. We show how to implement a simple precursor-flow shutter by changing the total pressure in the furnace reactor. This can be easily done for any vapour transport growth process in a quartz-tube and requires no mechanical parts. Once thermal gradients are eliminated, we show that the transition from one nanocrystal shape to another is controlled just by the interplay of precursor impinging on the substrate and sample surface kinetics [3]. In particular, a regime is found where seeded, epitaxial growth of CdSe nanorods becomes dominant over the conventional catalyst-assisted nucleation. This allows the fabrication of vertical nanorod arrays free of any metal contamination. Seeded growth of branched and tetrapod-like nanocrystals is also possible by further optimisation of the growth parameters.

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PTue 33

TRANSPARENT AND FLEXIBLE CARBON NANOTUBEA/ POLYPYRROLE SENSORS

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Thin film Carbon Nanotube (CNT) networks are used as a conductive, transparent and flexible electrode for electrochemically depositing a conducting polymer on it (1), polypyrrole in the present work. Conducting polypyrrole is reported to have different sensing properties: electrochemical or pH sensor (2), gas sensor for alcohol (3), NO2, chlorinated hydrocarbons, (4), biosensor (5). We analyse the properties of the device as electrochemical sensor, measuring his pH dependence by recording the open circuit potential in various buffer solutions ranging from pH 1 to 13, similarly to the recent reported results (6) on carbon nanotube/polyaniline pH sensors. The results show a good sensibility and linearity. The CNT/ polypyrrole devices can also have applications as solid state gas sensor or biosensor, that can be transparent and flexible, deposited on any shape of surface.

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PTue 34

PERCOLATED NETWORKS IN SWNT/POLYMER COMPOSITES: POLYMER DYNAMICS AND ELECTRICAL TRANSPORT

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SWNT/ PMMA nanocomposites were prepared by a coagulation method, providing uniform dispersion of the nanotubes in the polymer matrix. The linear viscoelastic behavior and electrical conductivity of these nanocomposites were investigated. At low frequencies the storage modulus G' is almost independent of frequency as the nanotube loading increases, suggesting an onset of solidlike behavior in these nanocomposites. By fitting G' vs. nanotube loading to a power law, a rheological threshold of these nanocomposites is identified at 0.12 wt %. This is less than the percolation threshold of electrical conductivity, 0.39 wt %. This difference in thresholds is understood in terms of the smaller nanotube-nanotube separation required for a percolated resistor network as compared to that required to impede polymer mobility [1].

Percolation conductivity of a network of conducting rods depends on alignment, or preferred orientation, as well as on concentration. We show that both dependences exhibit critical (power law) behavior, and study the orientational threshold in detail. We find, surprisingly, that the highest conductivity occurs for slightly aligned, rather than completely isotropic, rods. The experimental results from SWNT composites are fully borne out by Monte Carlo simulations [2].

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[2] F. Du et al., Physical Review B (in press).

PTue 35

The influence of monolayer surface passivation on transparent conductive oxide electrodes on the organic solar cell performance

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The charge transport properties at the interface between inorganic transparent conductive oxide (TCO) electrodes and organic films are crucial in organic optoelectronic devices. In order to improve charge carrier transition the TCO surface has to be adjusted. In the case of indium-tin-oxide (ITO) and metal phthalocyanines we propose to achieve this adjustment by chemical surface treatment of the ITO electrode. Both aromatic and acidic passivation by a molecular monolayer improves the performance of a phthalocyanine/C_{60} bilayer heterostructure solar cell significantly. By this procedure additional buffer layers can be substituted.

DFT investigation of doped molybdenum sulfide nanostructures

PTue 36

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Extended Chevrel-type molydenum sulfide nanostructures of the composition Mo:S = 3n:3n+2 exhibit pronounced Jahn-Teller distortions in the neutral state and a vanishing band gap with increasing n. The deviations from the ideal polyhedral shape maybe alleviated by electron doping. The present density-functional study exploits the influence of electron doping on the infinitely extended molydenum sulfide nanowire. The wire is composed of alternating Mo triangles, which are bridged by S atoms.Up to a doping level of m=3 electrons per Mo6S6 repeat unit the wire remains metallic and a Mo-d-based state crosses the Fermi level. Upon further doping to m=4 the system undergoes a metal-semiconductor transition. For higher doping levels m=5,6the system becomes metallic, again. As a realisation of this process, a decoration of the wire with Li atoms was investigated. Both the shift of Mo-d-based levels up to m=3 and the formation of a small gap at m=4 can be achieved by this decoration. At higher Li concentration of m=5,6 additional Li-based states contribute to the conductance channels in the vicinity of the Gamma point. Intratubular doping also leads to a participation of Li-based levels at the Fermi levels already at a lowerLi content of m=2. Yet, intratubular doping is geometrically restricted to m=1,2, thus the metal-semiconductor transition at m=4 can not be reached. Furthermore, the intratubular arrangement of Li causes considerable geometry changes, which make it less favourable than the extratubular decoration at S-bridging sites.

PERSPECTIVES FOR LOW-VOLTAGE ATOMIC-RESOLUTION TEM IMAGING OF BEAM SENSITIVE CARBON NANOSTRUCTURES

PTue 37

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A direct observation of the atomistic structure of carbon-based nanostructures like Nanotubes, Fullerenes, or Peapods by high-resolution transmission electron microscopy (HRTEM) is highly desired, but often hindered by radiation damage. Classical HRTEM instruments required high voltages of 200-300kV to obtain the necessary resolution in the range of 0.1nm. The corresponding energy of the electrons used for imaging are well above the damage threshold of the investigated carbon based structures, limiting severely the time-frame available for observation.

New instrumental developments promise to break this barrier and enable sufficient resolution even at acceleration voltages of 80kV, thus below the threshold energy of incident electrons on carbon atoms for atomic displacement damage. Especially the combination of a spherical aberration corrector for the objective lens and a monochromatic electron source should be able to achieve an interpretable resolution of 0.14nm in single shot images.

The expected information transfer and the impact on image resolution is discussed by transfer theory and HRTEM image simulation.of thight-binding optimized structures of nanotubes and peapods. The information transfer is compared to first test measurements.

Debundling of Single-Wall Nanotubes by Dilution: Observation of Large Populations of Individual Entities in High Concentration Dispersions

PTue 38

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Applications of single-wall carbon nanotubes (SWNT) are severely restricted,as they exist in rope-like bundles. Many methods have been suggested to de-bundle the SWNTs, including both covalent and non-covalent funtionalisation with surfactants, polymers and macromolecules. These methods have their advantages but the ideal situation must be to dissolve and de-bundle the SWNTs in an appropriate solvent at concentrations that are useful for their implementation in applications. In this work we have demonstrated debundling of single-wall nanotubes by diluting nanotubes dispersions in different amide solvents. Using Atomic Force Microscopy we observe the bundle diameter distribution to decrease dramatically with concentration. Near-infrared Absorption and Emission Spectroscopy were carried out on all solutions confirming an increase in the population of individual nanotubes with decreasing concentration.

PTue 39

Optimizing the growth of vertically aligned double-wall carbon nanotubes

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Carbon nanotube growth by chemical vapour deposition is carried out for two different catalyst preparation methods: a wet chemistry catalyst preparation is compared to a thin metal film multilayer catalyst preparation. As carbon sources alcohol and cyclohexane were used. The grown nanotubes are imaged by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Bulk properties such as diameters, yield and defect concentration are measured by optical absorption and resonance Raman spectroscopy. SEM images show dense mats of vertically aligned nanotubes of 0.1 mm length grown by cyclohexane on thin film multilayers. TEM micrographs show an abundance of nanotubes with 1-4 walls. Resonance Raman spectroscopy shows radial breathing modes for inner and outer nanotubes and low defect lines. Optical absorption spectroscopy shows that inner nanotubes have diameters between 0.6 nm - 1.3 nm and outer nanotubes have diameters from 1.3 nm - 2.0 nm. Yield determination by areal absorbances gives about 13 percent nanotube yield vs. impurities.

PTue 40

THE INFLUENCE OF GROWTH PARAMETERS ON DIAMETER OF SWCNTs IN ARC-DISCHARGE PROCESS

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A control of SWCNT diameters is required in some application. In this work we investigate the influence of growth parameters on the diameter of nanotubes in arc-discharge Krätschmer generator with horizontally aligned graphite electrodes. Various catalysts, buffer gases and additives were tested. We found that the pressure of buffer gas strongly affects the yield of SWCNTs, but it has only a small influence on the change of the diameter distribution. The catalysts composition and concentration of sulfur strongly influences the yield of SWNTs and change their diameter distribution. For Pt/Rh mixture, the mean diameter increases from 1.29 nm to 1.38 nm with increasing S concentration. The diameter distribution was narrowest for addition of 1.3 at% of sulfur. Various methods such as Raman and optical spectroscopy, TGA and TEM were used for characterization of products prepared at various growth conditions.

PTue 41

ORDERED INCLUSION OF N@C$_{60}$ AND P@C$_{60}$ IN A SINGLE-CRYSTALLINE MATRIX

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The pore-forming 2,4,6-tris(4-bromophenoxy)-1,3,5-triazine (BrPOT) was used to create a highly ordered self-assembled supramolecular arrangement of the endohedral fullerenes N@C$_{60}$ and P@C$_{60}$ in a single-crystalline host matrix. Two different guest-host structures were identified by x-ray diffraction and invesitgated by electron paramagnetic resonance (EPR). A uniaxial deformation of the fullerene guests leads to clearly resolved zero-field splitting of the quartet ground state of the encapsulated atoms, which is a useful property for quantum computing schemes.

HIGH-RESOLUTION PHOTOLUMINESCENCE IMAGING OF CARBON NANOTUBES PTue 42

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Near-field photoluminescence (PL) imaging of semiconducting single-walled carbon nanotubes (SWNTs) with a spatial resolution better than 15 nm is presented. Highly localized excitation of PL, provided by the enhanced fields at a laser-illuminated metal tip, is used to visualize the spatial extent of luminescent states along individual nanotubes. PL from micelle-encapsulated SWNTs on mica is typically extended along the nanotube up to several hundreds of nanometers. In some cases, a variation of the emission energy on a length scale of several 10 nm is observed. For SWNTs on glass, we detect highly localized PL from short segments of about 20 nm in length indicating bound excitons. The strong signal enhancement of PL results from enhanced excitation fields and an increase of the radiative rate in close proximity of the metal tip. Simultaneously acquired near-field Raman and PL data allows correlating local structural and luminescent properties of individual nanotubes.

Selective etching of metallic single-wall carbon nanotubes with hydrogen plasma PTue 43

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We present Raman scattering and scanning tunnelling microscopy (STM) measurements on hydrogen plasma etched single-wall carbon nanotubes (SWNTs). Interestingly, both the STM and Raman spectroscopy show that the metallic SWNTs are dramatically altered and highly defected by the plasma treatment. In addition, structural characterizations show that metal catalysts are detached from the ends of the SWNT bundles. For semiconducting SWNTs we observe no feature of defects or etching along the nanotubes. Raman spectra in the radial breathing mode region of plasma-treated SWNT material show that most of the tubes are semiconducting. These results show that hydrogen plasma treatment favours etching of metallic nanotubes over semiconducting ones and therefore could be used to tailor the electronic properties of SWNT raw materials.

Surface enhanced Raman spectroscopy of flat and curved carbon clusters PTue 44

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Hexa-perihexabenzocarbonate (HBC) are small cluster of a graphene plane with various side groups for stabilization. Due to their flat geometry they are ideal candidates to study surface enhanced Raman scattering (SERS).

Very thin films of HBCs were vapor deposited to different SERS-active Ag-surfaces. Thin films of Rodamine6G (R6G) were used as testing material for the SERS-effect. The enhancement of the Raman signal - which depends mostly on the surface-structure and is caused by electromagnetic (EME) and chemical enhancement (CE) - has been studied with the goal to develop an Ag-surface with maximum enhancement, for multiple use (SERS-chip) and to do reliable and efficent single molecule SERS. For the current surface the observerd surface enhancement is up to 10^6. For SWNT filled with Ag-particles the SERS-effect could also be shown - but enhancement is only a factor 10.

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PTue 45

CATALYTIC CVD OF SWNTS BELOW 400°C

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The catalytic nature of SWNT growth has been intensively studied in recent years, however, the detailed contributing processes remain disputed and not well understood. The high temperatures of bulk production techniques typically dominate growth model considerations. The vapor-liquid-solid (VLS) model suggested for silicon whisker growth is generally adopted to explain the growth of carbon SWNT, with the assumption that the catalyst cluster has to be in a molten state and bulk catalyst effects dominate the growth dynamics. These considerations are often also transferred to surface-bound CVD, carbon nanotube growth below 500°C is thought to be not possible based on calculations of size-corrected melting points and carbon saturation.

We report surface-bound growth of SWNTs at temperatures as low as 350°C by catalytic CVD from acetylene(1). This is the lowest temperature for SWNT growth reported to date, low enough to allow direct integration into back-end CMOS processing. Transistors based on our low temperature SWNTs show performances comparable to results on SWNTs grown at much higher temperatures. Subject to an appropriate catalyst film pre-treatment, carbon nanofibers can be nucleated at even lower temperatures, down to 200°C for purely thermal conditions. Our low temperature data challenges the commonly accepted growth model: based on ab-initio calculations(2) we suggest that carbon nanotube growth is governed by the catalyst surface without the necessity of catalyst liquefaction.

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PTue 46

ONE-DIMENSIONAL NANOSTRUCTURES SPONTANEOUSLY FORMED BY COMBUSTION SYNTHESIS

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The combustion synthesis is an efficient dehalogenation reaction of typical perhalogenated hydrocarbons. The heat generated by the exothermic process can be used to produce nanomaterials. We succeeded in sythesizing beta-SiC nanofibres and nanotubes via a spontaneous reaction of different alkyl and aryl halides with Si-containing reductants in a modified calorimetric bomb. The influence of the operating parameters on 1-D SiC formation yield was studied. The composition and structural features of the products were characterized by different techniques. This self-induced growth process can produce SiC nanofibres/nanotubes ca. 20-100 nm in diameter with the aspect ratio higher than 1000. Due to their high reflectivity single nanofibres, with a diameter up to 300 nm and length between 5 and 20 microns, were used as a resonant mass sensor (using a reflected laser beam to detect the oscillation). We also elucidate the nucleation V-L-S mechanism involving gaseous radicals responsible for 1-D nanostructure growth.

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AFM INVESTIGATIONS ON THE FORMATION OF 1-DIM STRUCTURES OF C_{60} SHUTTLECOCKS ON HOPG

PTue 47

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The arrangement of molecules on surfaces is a topic of interest for future electronic applications. Here, the formation of one-dimensional structures of chemically modified fullerenes on highly ordered pyrolytic graphite (HOPG) has been followed in situ with an atomic force microscope. The molecules used for the arrangement have the shape of a conical "shuttlecock" with a fullerene at the apex. Five biphenyl groups have been attached symmetrically around one C_{60} pentagon. The shuttlecock molecules where dissolved in toluene and spread on an HOPG substrate. Topographic images where taken with an atomic force microscope (AFM) operated in tapping mode. The formation of round islands, as well as needle shaped structures on the HOPG surface could be observed. The needles are only one monolayer high consistent with the formation of molecular chains. The observed width is compatible with 10 or less molecular rows. They arrange in three preferential directions probably due to the 3-fold symmetry of the graphite surface. By switching into contact mode one can manipulate and disrupt these chains. When switching back into tapping mode, one can observe their regrowth.

QUANTUM SUPERCURRENT TRANSISTORS IN CARBON NANOTUBES

PTue 48

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Electronic transport through nanostructures is greatly affected by the presence of superconducting leads. If the interface between the nanostructure and the superconductors is sufficiently transparent, a dissipationless current (supercurrent) can flow through the device due to the Josephson effect. A Josephson coupling, as measured via the zero-resistance supercurrent, has been obtained via tunnel barriers, superconducting constrictions, normal metals, and semiconductors. The coupling mechanisms vary from tunneling to Andreev reflection. The latter process has always occurred via a normal-type system with a continuous density of states. Here we investigate a supercurrent flowing via a discrete density of states, i.e., the quantized single particle energy states of a quantum dot, or artificial atom, placed in between superconducting electrodes. For this purpose, we exploit the quantum properties of finite-sized carbon nanotubes (CNTs). By means of a gate electrode, successive discrete energy states are tuned ON and OFF resonance with the Fermi energy in the superconducting leads, resulting in a periodic modulation of the critical current and a non-trivial correlation between the conductance in the normal state and the supercurrent. We find, in good agreement with existing theory, that the product of the critical current and the normal state resistance becomes an oscillating function, in contrast to being constant as in previously explored regimes.

DIRECT OPTICAL EXCITATION OF FULLERENE-INCARCERATED ERBIUM IONS

PTue 49

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$Er_3N@C_{80}$ is an endohedral fullerene that shows characteristic photoluminescent emission at 1.5 μm. At helium temperatures, the emission spectrum is sharply resolved and attributed to fluorescence from the Er^{3+} ion associated with radiative relaxation from the crystal-field split Er^{3+} $^4I_{13/2}$ manifold to the $^4I_{15/2}$ manifold. Previous observations of this luminescence have been carried out by photoexcitation of the fullerene cage states followed by nonradiative relaxation to the ionic states. Using a tunable 1.5 μm laser, we have been able to observe direct non-cage-mediated optical interactions with the erbium ion. This spectroscopic method provides the opportunity to map and study the energy level structure of the incarcerated ion and to use this information as a diagnostic of the ionic local environment and interaction with the cage.

PTue 50

QUANTITATIVE DETERMINATION OF DEFECT GROUPS AT SINGLE WALLED CARBON NANOTUBES VIA XPS

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Since the discovery of carbon nanotubes (CNTs) many efforts have been taken to take advantage of their unique mechanical and electronic properties. A large quantity of applications requires anchor sites for chemical functionalizations at the CNT-sidewalls which are most commonly introduced by oxidative treatment during the purification processes. A variety of functional groups (i.e. carboxyl, carbonyl, aldehyde, alcohol), representing the different oxidation states of carbon, can be produced in various amounts, depending on the time and the temperature of the process. For subsequent functionalization steps it is essential to know the quantitative amount of the functional group being converted in a chemical reaction. X-Ray Photoelectron Spectroscopy (XPS) proved to be a useful tool for such determination. Until today the asymmetry of the C1s core level in CNTs and the unknown peak positions of the functional groups prevented a detailed XPS analysis of the produced oxidized carbon species. In this work we present an effective method to overcome this problem using XPS combined with semi empirical calculations of the atomic charges in functionalized CNTs. It is shown that the peak positions of the functional groups can be calculated and that the resulting peak fits lead to a complete and quantitative analysis of the sample.

PTue 51

Microsystem design for TEM and Raman analysis from the same CNT

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Microchips realized from standard surface micromachining are used as a tool for the characterization of integrated carbon nanotubes. The CNTs are CVD grown inside a thin polysilicon grid which can be slided above the edge of the silicon chip thus becoming transparent and available for transmission imaging. The same chip containing identified CNTs can be used for further investigations in various other experimental setups and environments including SEM, Raman and electrical measurements.

PTue 52

THE INTERMEDIATE FREQUENCY MODES OF CARBON NANOTUBES: A RAMAN SPECTROSCOPIC AND IN-SITU RAMAN SPECTROELECTROCHEMICAL STUDY

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Raman spectroscopy is a preferred method to investigate carbon nanotubes (CNT) due to the resonant enhancement of the Raman signal. The main components of the spectra of CNT are radial breathing mode (RBM), tangential displacement mode (TG), disorder induced mode (D) and high frequency two-phonon mode (G'). There are additional bands in the region between 600 and 1100 cm-1 in the spectrum of CNT. Despite their importance for understanding CNT properties, only little attention was paid to this intermediate frequency mode (IFM) region. Here we present a study of this IFM features. The intermediate frequency modes of carbon nanotubes CNT were analyzed by Raman spectroscopy and in situ Raman spectroelectrochemistry. The data obtained by in situ spectroelectrochemistry support our studies of RBM, G and G' mode. The dependence of IFM on electrochemical charging is studied and discussed in detail. We have found that the nature of IFM bands has also an important impact on their charging behavior. The analysis of in-situ spectroelectrochemical data on CNT allowed more precise assignment of the bands in IFM region to features intrinsic for carbon nanotubes.

THE IMPACT OF SINGLE WALLED CARBON NANOTUBES ON HUMAN OSTEOBLASTS AND MESENCHYMAL STEM CELLS **PTue 53**

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Single-walled carbon nanotubes (SWCNTs) have many unique properties and therefore are also explored for application in biomedical engineering and medical chemistry. Such application requires the investigation of influence of carbon nanotubes and associated nanomaterials or nanodevices on human cells and environment.

In the present study we have investigated the influence of SWCNT on human osteoblasts (SAOS - tissue culture cell line) and mesenchymal stem cells (MSC - primary cells). The SWCNT were of the high quality as it was confirmed by Raman and UV-VIS-NIR spectroscopy. No surfactant has been used to minimize the effect of other agents on the behavior of the cells. In case of both cell types the covering of SWCNT with living (proliferating) cells was observed. Nevertheless the results also showed that SWCNTs has significant effect on cell metabolism of both cell types. The osteoblasts metabolic activity was decreased by 15% independently on the amount of cells used. The metabolic activity of mesenchymal stem cells was dependent on the used cell number. The drop of activity varied between 15 and 25%. The higher the cell amount was used the smaller decrease in activity was observed. Thus our results demonstrated that SWCNTs exhibit the slightly reduced biocompatibility with respect to investigated human cells.

POLARIZATION-DEPENDENT OPTICAL REFLECTIVITY IN MAGNETICALLY ORIENTED CARBON NANOTUBE NETWORKS **PTue 54**

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We will present the optical spectra of carbon nanotube networks, oriented in a magnetic field, in a wide frequency range from the far infrared through the visible. In the far infrared, the absorption of the metallic tubes is clearly preferred in the polarization parallel to the tube axes, with intensity ratio 2:3 between reflectance perpendicular and parallel, respectively. Strong polarization dependence also occurs for symmetric transitions between the first Van Hove singularities of the semiconducting tubes; however, we detect a strong peak in the near infrared polarized perpendicular to the alignment direction. We will discuss the possible origins of this peak: asymmetric transitions allowed for perpendicular polarization, preferred alignment by chirality or optical resonance processes.

RAMAN SPECTROELECTROCHEMISTRY OF INDEX-IDENTIFIED CARBON NANOTUBES **PTue 55**

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Raman spectroelectrochemistry of single- and double-walled carbon nanotubes (SWCNT, DWCNT) was studied at conditions, when the radial breathing modes (RBM) can be assigned to defined chiralities from the experimental Kataura plot. The particular (n,m) tubes exhibit different sensitivity to electrochemical doping, monitored as an attenuation of the RBM intensities. Tubes, which are in optimum resonance with the exciting laser, exhibit the strongest doping-induced drop of the RBM intensity and vice versa. This simple rule asks for re-interpretation of some earlier results about the diameter-selectivity of doping. The precise distinction of tubes, which are in good resonance, from tubes, which are in weaker resonance with the exciting laser, presents a tool for analysis of mixture of nanotubes of unknown chiralities. Our ”resonance rule” is particularly important for the investigation of inner tubes in DWCNT and for metallic tubes, which cannot be indexed from the experimental Kataura plot.

PTue 56

PHOTOLUMINESCENCE MICROSCOPY ON AS-GROWN INDIVIDUAL SINGLE-WALLED CARBON NANOTUBES

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We present far-field photoluminescence (PL) imaging at room temperature of tens of micrometer long individual single-walled carbon nanotubes (SWNTs) grown and measured directly on a silicon oxide surface. The SWNTs are grown by Chemical Vapour Deposition (CVD) with ethanol as carbon source and contact the surface with their full length. We detect the PL and its variations along the tube with a resolution of ≈400 nm. We are able to reliably assign (n,m) by measuring PL spectra in the range of 800-1600 nm as a function of the excitation wavelength varying between 710 and 860 nm. This allows us to detect changes of chirality along the tube.

PTue 57

Electric Transport Properties and NMR Study of the Fullerene-Like WS2 Nanoparticles

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Electrical resistivity and Hall measurements, of pellets compacted from IF-WS2 nanoparticles and 2H-WS2 powder were done. Electrical transport measurements were carried out on pellets by the van der Pauw method in a wide temperature range. Arhhenius plots for conductivities of the WS2 samples (2H, IF and IF+treatment) are curved. Resistivity of IF-WS2 pellets is higher than that of 2H-WS2 pellets. It was found that the electrical properties of IF-WS2 powder depend on the treatment. The NMR measurements show that the prepared product contains water (and possibly some hydrogen) molecules that occupy the voids in the central part of the fullerene-like nanoparticles and the nanopores between the adhering IF-WS2 particles. Defects in the IF-WS2 structure, arising due to the strain release during the folding of the layers, may result in additional sites for the absorbed water.

PTue 58

TOPOCHEMICAL COPOLYMERIZATION OF FULLERENES WITH CUBANE IN THEIR ROTOR-STATOR PHASES

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A new family of heteromolecular crystals has been described recently: the rotor-stator phases of fullerenes with cubane. Cubane, the stator component of these materials is a highly strained molecule which decomposes to higher stability C8H8 hydrocarbons at 500K. This unimolecular isomerization takes also place in the rotor-stator phases, inducing a single phase topochemical reaction with the surrounding fullerenes. The resulting material is a random copolymer, percolating in the primitive cubic sublattices of the parent crystals. We followed the polymerization by HPLC, IR and UV-VIS spectroscopy and optical microscopy, and determined the thermal stability by TG-MS analysis. The polymers are insoluble, and stable up to 700K. At this temperature they start to decompose while preserving their crystalline appearance. The influence of the side groups of substituted cubanes on the polymerization will also be discussed.

PTue 59

Isotope Engineered Synthesis and Characterisation of Single Wall Carbon Nanotubes

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We report on the optimised synthesis of high quality isotope engineered SWCNT by means of laser ablation and the use of Pt-Rh-Re catalyst mixtures. Optical absorption and multifrequency Raman spectroscopy as well as transmission electron microscopy are utilized to characterize the obtained SWCNTs. The yield and diameter distribution are proven to be stable and reproducible. The absence of any ferromagnetic materials, as well as the remarkably low abundance of amorphous carbon renders this material ideal for electron spin resonance. The controlled augmentation of ^{13}C is conveniently confirmed by phonon softening and broadening observed via Raman spectroscopy.

PRESSURE-DEPENDENT INFRARED SPECTROSCOPY ON THE FULLERENE ROTOR-STATOR COMPOUND C_{60}-C_8H_8

PTue 60

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The recently synthesized fullerene-cubane molecular crystals constitute rotor-stator systems, where the static cubane, C_8H_8, occupies the octahedral interstices of the face-centered-cubic structure and acts as a bearing between the rotating fullerene molecules [1]. C_{60}-C_8H_8 undergoes a structural phase transition at around 140 K, where the rotation of the fullerenes stops. This transition temperature is significantly lower than in any other fullerene derivative due to the increased free volume between the fullerene molecules. Accordingly, at room temperature a pressure-induced orientational ordering transition is expected to occur at higher pressures compared to, e.g., solid C_{60}.

We carried out infrared transmission measurements of C_{60}-C_8H_8 as a function of pressure (0-10 GPa). The kinks in the pressure dependences of the frequencies of the molecular vibrations suggest the occurrence of an orientational ordering transition at 0.7-0.8 GPa at room temperature. Furthermore, our data show that the vibrations of C8H8 survive up to a higher pressure than those of C_{60}, indicating the shielded positions of these molecules in the crystal. The pressure-induced changes of the properties will be compared to the changes as a function of temperature.

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DOUBLE-WALLED CARBON NANOTUBE WITH THE SMALLEST INNER DIAMETER: AN AB INITIO STUDY

PTue 61

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The smallest diameter “inner tube” in a double-walled carbon nanotube is the linear carbon chain. Long linear carbon chains in multi-walled carbon nanotubes have been observed experimentally using electron microscopy and Raman spectroscopy [1,2]. We have studied the geometry and the electronic stucture of the combined system (infinite long chain -polyyne- in carbon nanotubes with various chiralities) by DFT method [3]. The frequency of the longitudinal optical mode of polyyne is usually assumed to be at around 2000-2200 cm-1. We have carried out careful analysis introducing a novel linear/exponential scaling to correctly treat the long-range coupling for off-diagonal force constants [4]. With this new scaling scheme, the frequency of the Raman active mode of polyyne was determined to be 1877 cm-1. This value combined with the effect of charge transfer between the chain and the tube offers a possible interpretation for the Raman band observed at around 1850 cm-1 in the combined system [2].

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PTue 62

Simultaneous dispersion and ordering of carbon nanotubes in a self-organizing lyotropic liquid crystalline matrix

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In many projected applications of carbon nanotubes (CNTs) high performance requires large-scale uniform alignment of the tubes. For tubes detached from the growth substrate this requirement is intimately coupled with the need for efficient dispersion, i.e. the tendency for flocculation into disorganized bundles must be overcome. The most successful approach is to keep the nanotubes in low-concentration surfactant+water solutions, the surfactant often being sodiumdodecylsulfate (SDS). At higher concentrations such solutions form lyotropic liquid crystal (LC) phases. LCs have turned out to be highly useful hosts for aligning CNTs but so far only thermotropic LCs have been investigated.

We here study lyotropic LC hosts for simultaneous dispersion and alignment of HiPCO single-wall CNTs. As the phase diagram of a lyotropic system critically depends on mixture composition, the first challenge was to identify a host that supports the presence of nanotubes and at the same time ensures an efficient dispersion. Using quaternary CNT+SDS+decanol+water mixtures we achieved good long-term (several months) CNT dispersion in a nematic phase (orientational but no translational order) which is thermodynamically stable at room temperature. The nematic phase was not disrupted with CNT concentrations as high as 1 mg/mL. Quantitative analysis of the alignment efficiency is currently in progress.

PTue 63

Geometric and electronic structure of carbon nanotube junctions

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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. The rolling up of the graphene changes, however, the angles and distances between the carbon atoms in the hexagonal network and in a more sophisticated calculation curvature effects and the corresponding hybridizations must be taken into count. The electronic structure is modified also by possible non hexagonal polygons in the hexagonal network. This is the case if we study the electronic properties of a nanotube junction. Nanotube junctions are possible candidates for building blocks in nanoscale electronic devices and in an ideal case each nanotube junction must contain at least six heptagons if other polygons are not allowed. If the chirality of the tubes of a junction is given there are also various possibilities for the positions of the heptagons and each of them must have different electronic properties. In this work the connection between the geometric and electronic structure of a junction will be studied using various tight-binding methods.

PTue 64

Functionalization of Single-Walled Carbon Nanotubes by Aromatic Molecules Studied by Scanning Tunneling Microscopy

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A functionalization of single-walled carbon nanotubes (SWCNTs) without the necessity to introduce defects to the atomic structure of the graphitic lattice can be achieved via pi-stacking interaction of the SWCNTs sidewalls with aromatic molecules. In our work we study the functionalization of SWCNTs with different aromatic molecules, e.g. aminoanthracene, by scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS).

Functionalization was performed in solution and the SWCNTs so obtained were transfered to a sputter-annealed Au (111) substrate using dry transfer techniques in vacuum to avoid surface contamination by ambient air. STM measurements were carried out at 77 K and 4.7 K in ultrahigh vacuum. Differential conductance imaging of the atomically resolved functionalized SWCNTs reveals a substructure which can be attributed to the molecular orbitals of the aromatic molecules. These findings are compared to the STM images obtained from the bare molecule prepared by thermal evaporation on a clean Au (111) surface which are interpreted with the help of quantum chemical calculations of the molecular orbital structure.

COMPARATIVE STUDY STRUCTURAL-VIBRATIONAL IN THE FORMATION OF NANOURCHIN AND NANORODS OF VANADIUM PENTOXIDE

PTue 65

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Vanadium oxide based nanotubes (VONTs) and nanofibers have been studied extensively for their optical and electrical properties [1] and their application as components of gas sensors has been explored [2]. However the new kind of nanostructures like nanourchin and nanorods of this transition element oxide was synthesised [3] with present potential applications.

In this since, it was synthesised vanadium oxide nanourchin (VONURs) with 9-12 mm of diameter and vanadium oxide nanorods (VONRs) with 200-100 nm of diameter [3]. The HR-TEM of the VONURs show that 2.85 nm is the interlamellar distance of the vanadate units, as well it was found that the surfactant inside is in "all-trans" configuration.

In this work we present a discussion of the vibrational (Raman, FTIR) and, structural (HR-TEM) comparative study between the VONURs, that present mainly the a-V2O5 structure and, the vanadium oxide nanorods (VONRs) with 200-100 nm of diameter, where the vibrational spectra suggest that the V4+ specie is present in minor quantitative.

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MECHANICO- CHEMICAL INTERACTION OF SWNTS WITH DIFFERNT HOST MATRICES EVIDENCED BY SERS SPECTROSCOPY

PTue 66

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Surface enhanced Raman scattering (SERS) at 676.4 and 1064 nm excitations were used to investigate single-walled carbon nanotubes (SWNTs) thin films prepared from platelets obtained by non-hydrostatic compression at 0.58 GPa. SWNTs were compressed alone or dispersed into chemical reactive and non-reactive host matrices. SiO2 and Al2O3 as non-reactive host matrices and inorganic compounds (KI and Ag microparticles) and aromatic hydrocarbons (AHs) as reactive host matrices were used. SERS spectra indicate that by compression, SWNTs break into fragments of different sizes, which in turn can react or not with the host matrix. In inorganic hosts (KI, Ag) donor-acceptor complexes are formed. Regardless AHs type used, i.e. with isolated (biphenyl, p-terphenyl) or condensed (naphthalene,phenantrene) phenyl rings, a non-covalent functionalization of SWNTs and their fragments is produced. An ionic and covalent functionalization of unbroken and broken SWNTs is demonstrated when AHs with isolated phenyl rings, i.e., biphenyl or p-terphenyl, are used as host matrices. The appearance of short fragments of SWNTs with a closed-shell fullerenes behaviour is revealed both in SERS and photoluminescence spectra. This typical signature appears in the Raman spectrum as a line at ≈ 1460 cm-1 associated with a pentagonal pinch mode. Additional proofs are given by TEM images.

PTue 67

ELECTRICAL MEASUREMENTS ON DEVICES FABRICATED WITH SUB-NM SIZED MOLECULES

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[1]Nanotechnology Research Institute, AIST, and JST-CREST, Japan; [2]Korea Research Institute of Chemical Technology; [3]Kavli Institute of Nanoscience, TU Delft, Netherlands

In order to measure the electrical properties of single molecules or other small nano-objects like metal clusters, the ability to apply a gate voltage is of paramount importance. In the past few years, considerable efforts have been put into fabricating electrode pairs with nanometer-sized gaps on top of a back-gate. Methods that have been employed include electromigration, electrochemical etching, and shadow-evaporation. In this work, we have fabricated shadow-evaporated electrodes that exhibit a wide range of linear tunnel resistances. Upon self-assembling two kinds of sub-nanometer sized molecules on them we obtained different transport characteristics. While one type of molecule just led to decreased, non-linear tunnel resistances with occasional peaks in the differential conductance, the other type of molecule led to a plethora of highly correlated, gate-dependent transport characteristics indicating Coulomb blockade, elastic and inelastic co-tunneling, charge reconfiguration and peaks in the differential conductance near zero bias.

PTue 68

SIDEWALL FUNCTIONALIZATION OF SINGLE-WALLED CARBON NANOTUBES BY ORGANO-METALLIC MOLYBDENUM-CENTERED FREE RADICALS

A.S. Lobach[1], A.P. Dementjev[2], E.D. Obraztsova[3], R.G. Gasanov[4], and V.I. Sokolov[4]
[1]Institute of Problems of Chemical Physics RAS, 142432 Chernogolovka, Moscow Region, Russia; [2]Russian Research Centre "Kurchatov Institute", Kurchatov sq. 1, 123182, Moscow, Russia; [3]Natural Sciences Center of General Physics Institute, RAS, 38 Vavilov Street, 119991 Moscow, Russia; [4]Nesmeyanov Institute of Organoelement Compounds RAS, 28 Vavilov

Chemical functionalization of single-wall carbon nanotubes (SWNT) is very important for development technological applications of nanotubes. The present work reports on investigations of interaction process of SWNT-HiPco with organometallic molybdenum-centered free radicals (Mo-CFR) generated by the homolytic dissociation of (cyclopentadienyl) molybdenumtricarbonyl dimer, ([CpMo(CO)3]2 in toluene at ultraviolet irradiation. The interaction of Mo-CFR with SWNT-HiPco and fullerene C_{60} in toluene was investigated using ESR spectroscopy. The material of Mo-CFR functionalized SWNT were successively characterized using UV-vis-NIR, XPS and Raman spectroscopy and TGA. It was demonstrated that the addition of Mo-CFR to SWNT without changing the type of hybridization of surface carbon atoms of nanotubes. The compounds can be considered as those having an ionic bond formed between a molybdenum complex and a carboxyl group of oxidized SWNT-HiPco.

PTue 69

Laser-assisted electron emission from CVD nano-graphite films

D. A. Lyashenko[1,2], E. D. Obraztsova[2], A. N. Obraztsov[3], and Yu. P. Svirko[1]
[1]Department of Physics, University of Joensuu,Yliopistokatu, 7, Joensuu, 80101, Finland; [2]Natural Sciences Center of General Physics Inst., RAS, 38Vavilov street, 119991, Moscow, Russia; [3]Physics Department of Moscow State University, 119992, Moscow, Russi.

Nano-carbons have recently emerged as promising materials for manufacturing high-efficient field-emission cathodes. In this work we demonstrate that CVD nano-graphite films produce also a strong electron emission under irradiation with nanosecond light pulses.

Nano-carbons have recently emerged as promising materials for manufacturing high-efficient field-emission cathodes. In this work we demonstrate that CVD nano-graphite films produce also a strong electron emission under irradiation with nanosecond light pulses.

In the experiment, we measured electron emission form the nano-graphite cathode as a function of the applied voltage and the power of the incident laser pulse (wavelength is 1600nm, pulse is 10 ns long, laser spot size of 7 mm2). We demonstrate that the threshold laser intensities for the laser-assisted electron emission from the nanographite decreases from I = 18 MW/cm2 at the cathode-anode electric filed E = 0,005 MV/m to I = 16 MW/cm2 at E = 2 MV/m, while the temporal profile of the obtained emission current reproduces the shape of the laser pulse. The current density of 7 A/cm2 was achieved at the laser intensities of I = 26 MW/cm2. The obtained dependence of the emission current of the pulse intensity and applied field enables us to perform a comparative study of the laser-assisted and field electron emission from nano-graphite in terms of work function and local field enhancement factor.

Template grown nanomaterials

8:30 – 9:00 K. SUENAGA, JP
HR-TEM imaging of molecules and ions trapped inside carbon nano-spaces

9:00 – 9:30 J. SLOAN, UK
Structural correlation of band-gap modifications induced in mercury telluride by dimensional constraint in single walled carbon nanotubes

9:30 – 10:00 R. PFEIFFER, A
Tube-tube interaction in template grown single wall carbon nanotubes

10:00 – 10:30 Coffee break

10:30 – 11:00 H. ALLOUL, F
NMR evidence for uniform electronic properties in a macroscopic set of DWCNT

COMMERCIALS

11:00 – 11:30 L. FORRÓ, CH
Conduction electron spin resonance of single wall carbon nanotubes

11:30 – 12:00 F. SIMON, HU
$C_{59}N$ monomer spins inside single-wall carbon nanotubes: rotational dynamics, charge transfer, and local density of states.

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

Nanomechanics

18:30 – 19:00 P. RUDOLF, NL
Macroscopic transport by synthetic molecular machines

19:00 – 19:30 J.C. MEYER, D
Nano-electromechanical devices based on single-walled carbon nanotubes

19:30 – 20:00 S. PEKKER, HU
Rotor-stator phases of fullerenes with cubane derivatives: A novel family of heteromolecular crystals

Celebration 20th IWEPNM

20:10 – 20:50 M. MEHRING, D
Twenty International Winterschools in Kirchberg: How come?

20:50 – 21:40 S. IIJIMA, JP
Nano-carbon materials: formation, characterization, and applications

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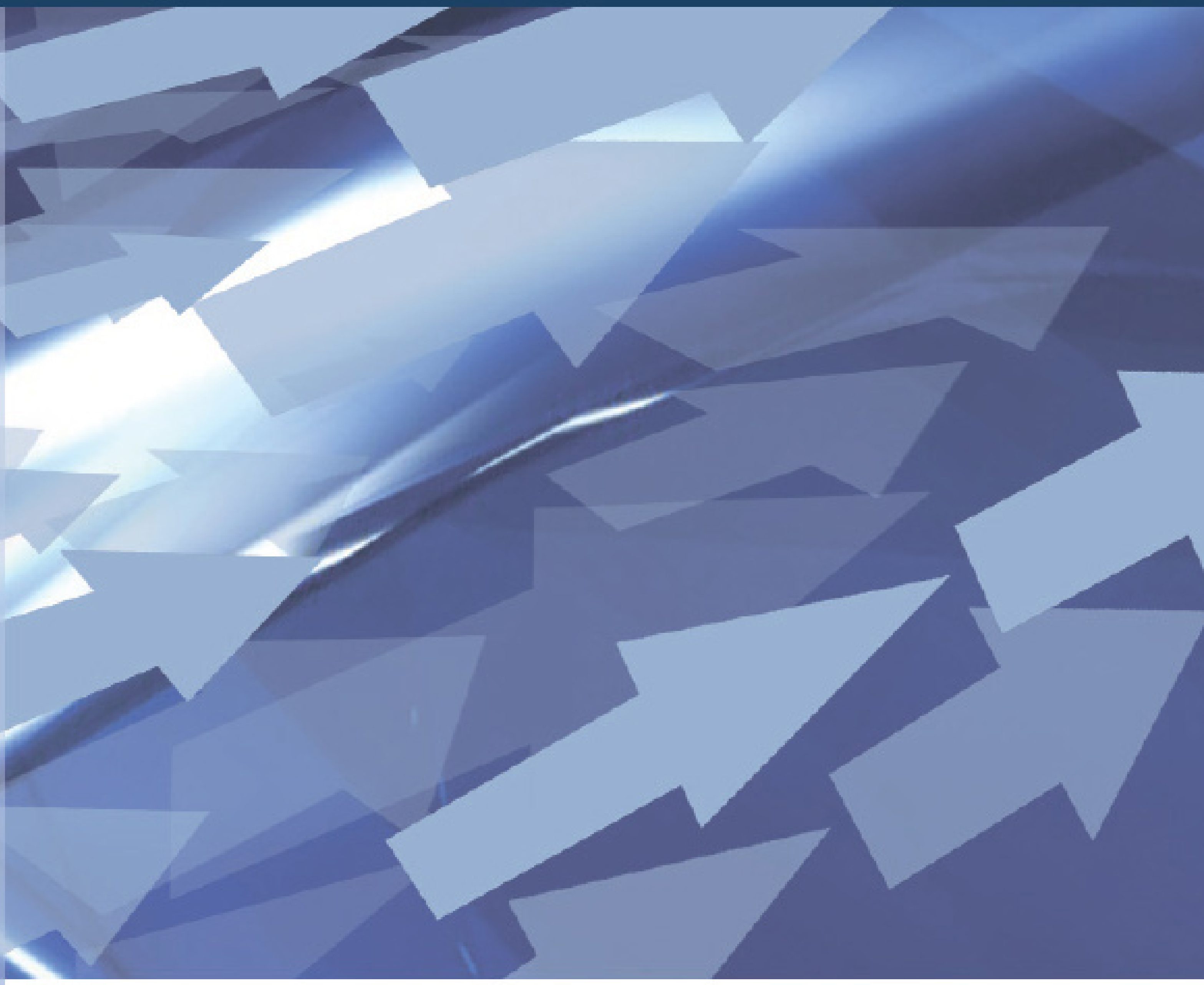

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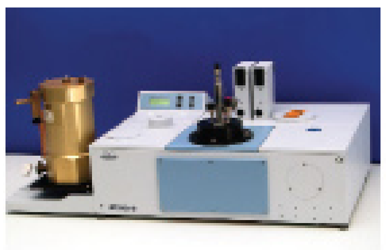

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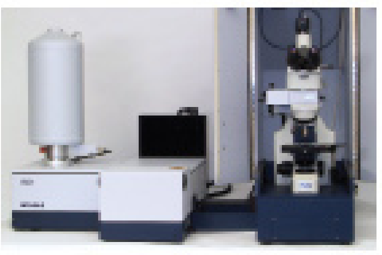

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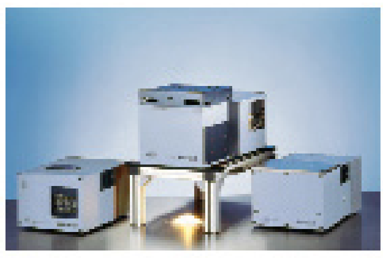

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HR-TEM imaging of molecules and ions trapped inside carbon nano-spaces

8:30 TGNM 1

Kazutomo Suenaga
AIST, Tsukuba, Japan

Carbon materials have long been known to possess "nano-spaces," where a variety of materials can be stored. In order to reveal the storing mechanisms of carbon nano-spaces we have tried to use the high-resolution transmission electron microscopy (HR-TEM) to visualize various molecules and ions trapped inside porous nano-carbon materials. Attempts to encapsulate various fullerene molecules and alkali metals inside the carbon nanotubes and/or nanohorns were made. Results will provide direct identification of the preferable adsorption sites for examined molecules and atoms.
Supported by NEDO and JST. Collaboration with Peking Univ., Nagoya Univ., and Tokyo Univ.

Structural correlation of band-gap modifications induced in mercury telluride by dimensional constraint in single walled carbon nanotubes

9:00 TGNM 2

J. Sloan, R. Carter, R.R. Meyer, A. Vlandas, A.I. Kirkland, P.J.D. Lindan, G. Lin, J. Harding, J.L. Hutchison, and M.L.H. Green
University of Oxford, Universiy of Kent, University of Sheffield

In this abstract we describe a unique structure for HgTe grown inside narrow single wall carbon nanotubes (SWNTs) based on a repeating Hg_2Te_2 atomic motif with both atom species in novel coordination geometries. Two unique projections were obtained by high resolution transmission electron microscopy from two separate encapsulated crystal fragments enablingre construction of a three dimensional arrangement of atoms within the two encapsulated fragments. The observed structure was separately determined by quantum mechanical calculations that confirm the global stability of the HgTe structure and demonstrate conclusively that it arises solely as a consequence of its constrained, low-dimensionality. We have also calculated that this structural change is correlated directly with a fundamentally modified electronic structure resulting in the transformation of HgTe from the bulk semimetal to a semiconductor when confined within a SWNT.

Tube-tube interaction in template grown single wall carbon nanotubes

9:30 TGNM 3

Rudolf Pfeiffer[1], Ferenc Simon[1], Christoph Schaman[1], Hans Kuzmany[1], V.N. Popov[2], Viktor Zólyomi[3], Jenő Kürti[4], and R. Herges[5]
[1]Institut für Materialphysik, Universität Wien, Austria, [2]Faculty of Physics, University of Sofia, Sofia, Bulgaria, [3]MTA-SZFKI, Budapest, Hungary, [4]Dept. of Biol. Phys., Eotvos University Budapest, Hungary, [5]Institut für Organische Chemie, Universität Kiel, Germany

We present resonance Raman studies on C_{60} peapod grown double-wall carbon nanotubes (DWCNTs) using an almost continuous excitation between 1.52 and 2.71 eV. Due to the very narrow linewidths of the radial breathing modes (RBMs) of the inner tubes, these experiments revealed clear patterns for tube families of different tube types (metallic and semiconducting type I and II) which allowed a full chirality assignment for each tube and transition. Additionally, the RBMs of the inner tubes are grouped into clusters close to the response of SDS dispersed HiPco tubes (R. Pfeiffer et al., PRB 72, 161404(R) (2005)). Every cluster originates from one specific inner tube in several but well-defined outer tubes where every inner/outer tube pair contributes one RBM peak. The half-widths of the Raman cross-sections of the inner tubes of bucky-paper DWCNTs are similar to that of SDS dispersed SWCNTs and significantly smaller than for buck-paper SWCNTs, although they show a similar temperature dependence.
The tube-tube interaction results in a downshift of transition energies which leads in many cases to a closure of the gaps. Such behavior is consistent with recent NMR studies on ^{13}C peapod-grown DWCNTs where evidence is provided for a metallic state of the inner tubes (P.M. Singer et al., PRL 95, 236403 (2005)).
Tube-tube interaction can also lead to structural transformations of interacting molecules. This will be discussed for the case of picotubes (anthracen tetramer) interacting with NT bundles.
Work supported by FWF project No. P17345 in Austria and Marie-Curie Project Nos. MEIF-CT-2003-501099 and MEIF-CT-2003-501080, and by NATO CLG 980422.

10:30
TGNM 4

NMR evidence for uniform electronic properties in a macroscopic set of DWCNT

P. Singer, P. Wzietek, H. Alloul, F. Simon, and H. Kuzmany
Physique des Solides Osray, France

Single-wall carbon nanotubes (SWNT) are expected theoretically, and found experimentally to display enormous differences in electron transport behaviour, from metallic to large gap insulator, depending upon their diameter and the way the constituting hexagonal graphene foil is rolled. Recently double wall carbon nanotubes (DWCNT) have been synthetized by filling SWNT with fullerenes (so called "peapods") and high T reaction which merges the fullerenes into inner tubes. Those DWCNT have some exceptional properties as the inner tubes are accommodated in a highly shielded environment under clean room conditions.

In this report the possibility to achieve selective enrichment of the inner shells by using 13C isotope enriched fullerenes [1] in the peapod synthesis, has been used to probe by 13C nuclear magnetic resonance the specific properties of he inner tubes. We find [2] that, although distributed in diameter and chirality, these inner tubes display strikingly homogeneous electronic properties. We evidence , from the study of the 13C nuclear spin dynamics, that the magnetic properties of the inner tubes behave as expected for a one dimensional metallic chain at room T, but exhibit a sharp gap (of the order of 20K) at low T. This unexpected quasi uniform behaviour displayed by this specific macroscopic collection of nanotubes should stimulate further experimental and theoretical investigations. It opens for the first time the possibility to study physical properties on macroscopic samples of nanotubes.

[1] F. Simon et al, Phys. Rev. Lett. 95, 017401 (2005).
[2] P. Singer et al, Phys. Rev. Lett. 95, 236403 (2005).

11:00
TGNM 5

Conduction electron spin resonance of single wall carbon nanotubes

Titusz Fehér, Balint Náfrádi, Lecoultre Sylvain, Ferenc Simon, Hans Kuzmany, and László Forró
Institute of Physics of Complex Matter, EPFL, Lausanne, Switzerland

Conduction electron spin resonance (CESR) as a very sensitive tool can give a direct information on the electronic properties of single-walled carbon nanotubes(SWNTs). However, this sigmnal has not been observed yet. We believe this is due impurities, like catalytic particle, which smear out the inherent CESR signal. As recently discovered, good quality DWNT-s can be synthesized by a simple heat treatment from peapods1 as the C60 molecules fusion at high temperature into very clean, small diameter nanotubes. The outer nanotube – as a shell – could provide a sort of protection case from the environment for the inner tube, it can inhibit the electrons to diffuse to the catalytic particles. Moreover, the inner nanotubes are also protected from atmospheric oxygen adsorption having a profound effect on their electronic properties. We report on a series of carefully executed ESR experiments on peapod samples annealed at various temperatures.

Acknowledgment: This work is supported by the TMR Network “NANOTEMP” of the European Community.

1. S. Bandow et al., Chem. Phys. Lett. 337, 48 (2001).

$C_{59}N$ monomer spins inside single-wall carbon nanotubes: rotational dynamics, charge transfer, and local density of states.

11:30 TGNM 6

F. Simon[1], H. Kuzmany[2], B. Náfrádi[3], T. Fehér[2], L. Forró[2], F. Fülöp[3], A. Jánossy[3], F. Hauke[4], and A. Hirsch[4]

[1] Institut für Materialphysik, Universität Wien, Strudlhofgasse 4, A-1090 Wien, Austria [2]Institute of Physics of Complex Matter, FBS Swiss Federal Institute of Technology (EPFL), CH-1015 Lausanne, Switzerland [3] Budapest University of Technology and Economics, Institute of Physics and Solids in Magnetic Fields Research Group of the Hungarian Academy of Sciences, H-1521, Budapest P.O.Box 91, Hungary [4] Institut für Organische Chemie der Friedrich Alexander Universität Erlangen-Nürnberg. Henkestrasse 42, D-91054 Erlangen

Filling of single-wall carbon nanotubes with $C_{59}N$ azafullerene derivatives is reported from toluene solvent at ambient temperature. The filling is characterized by high resolution transmission electron microscopy and Raman spectroscopy. The filling efficiency is the same as for C_{60} fullerenes and the tube-azafullerene interaction is similar to the tube-C_{60} interaction. Vacuum anenaling removes the sidegroup and the electron spin resonance (ESR) signal of $C_{59}N$ radicals is observed after vacuum annealing. The temperature dependent ESR spectra indicates a strongly hindered and non three-dimensional rotation of $C_{59}N$. The shortening of spin-lattice relaxation time, T_1, of $C_{59}N$ indicates a reversible charge transfer toward the nanotube above $\approx 550\,K$. At low temperatures, bound $C_{59}N$-C_{60} heterodimers are formed such as in crystalline $C_{59}N$: C_{60}. The temperature dependence the heterodimer T1 indicates a relaxation dominated by the SWCNT conduction electrons.

This work was supported by the Austrian Science Funds (FWF) project Nr. P17345, by the Deutsche Forschungsgemeinschaft (DFG), by the Hungarian State Grants (OTKA) T043255 and TS049881 and by the EU projects NANOTEMP BIN2-2001-00580.

18:30
NME
1

Macroscopic transport by synthetic molecular machines

Petra Rudolf
Materials Science Centre, Rijksuniversiteit Groningen, Nijenborgh 4, 9747 AG Groningen, NL

Biological motors are capable of transporting objects many times more massive than themselves and have been used to power prototypical hybrid mechanical devices. However, performing macroscopic mechanical tasks with the early generations of wholly synthetic molecular machines has proved more elusive. Here we shall report on the macroscopic (millimeter scale) transport of a droplet on a photo-responsive surface created using the nanometer displacement of the components of light-switchable molecular shuttles to expose or conceal fluoro-alkane residues and thereby modify surface tension or wettability of the surface. Stimuli-responsive molecular shuttles are rotaxanes in which the macrocycle can be translocated from one position ('station') on the thread to a second site through an external trigger (e.g. light, electrons, temperature, pH, nature of the environment, reversible covalent bond formation etc.). When the rotaxanes are grafted onto the surface and a drop is deposited on this surface, one can change the wettability of the surface in front of the drop by light-induced movement of the macrocycles. The collective operation of a monolayer of the shuttles is sufficient to power the movement of a microlitre droplet of diiodomethane up a twelve degree incline.

19:00
NME
2

Nano-electromechanical devices based on single-walled carbon nanotubes

Jannik C. Meyer[1], D. Obergfell[1], M. Paillet[2], T. Michel[2], J.-L. Sauvajol[2], and S. Roth[1]
[1] Max Planck Institute for Solid State Research, Stuttgart, Germany
[2] Laboratoire des Colloides, Verres et Nanomateriaux, Universite de Montpellier II, France

We have built mechanical devices based on individual single-walled carbon nanotubes. A metal plate, large enough to be visible in an optical microscope, is attached to a nanotube which serves as a torsional spring and mechanical support [1]. The electric field from a nearby electrode is used to turn the plate, and thereby twist the nanotube. The device could be used as actuator in a nanoelectromechanical system (NEMS), or as a very sensitive nanoscale sensor. For investigating our carbon nanotube based devices we prepare them in such a way that a TEM and electron diffraction analysis is possible [2]. Electron diffraction analysis of a torsionally deformed carbon nanotube facilitates a determination of its indices and in addition its handedness.

With a similar approach we have also obtained a combination of Raman spectroscopy [3] or transport measurements [4] with TEM and electron diffraction on the very same SWNT.

[1] J.C. Meyer et al., Science 309 p. 1539 (2005)
[2] J.C. Meyer et al., Ultramicroscopy, In Press (available online)
[3] J.C. Meyer et al., Phys. Rev. Lett. 95 p. 217401 (2005)
[4] J.C. Meyer et al., Appl. Phys. Lett. 85 pp. 2911-2913 (2004)

19:30
NME
3

Rotor-stator phases of fullerenes with cubane derivatives : A novel family of heteromolecular crystals

S. Pekker[1], É. Kováts[1], G. Oszlányi[1], G. Bényei[2], G. Klupp[1], G. Bortel[1], I. Jalsovszky[2], E. Jakab[3], F. Borondics[1], K. Kamarás[1] and G. Faigel[1]
[1] Research Institute for Solid State Physics and Optics, HAS. H-1525 Budapest, P.O.Box 49, Hungary;
[2] Department of Organic Chemistry, Eötvös Loránd University H-1518 Budapest, P.O.Box 32, Hungary;
[3] Chemical Research Center, HAS. H-1525 Budapest, P.O.Box 17, Hungary

We present the formation, structure and properties of a new family of molecular crystals of distinct rotating and static components: the derivatives of fullerenes with cubane. The new crystals consist of alternating arrays of the constituents, stabilized by the recognition of the complementary molecular surfaces. The concave cubanes match six rotating fullerenes in octahedral configuration, while the six nearest neighbours of the convex fullerenes may form either octahedral or trigonal prismatic configurations. Fullerenes rotate freely in the "molecular bearing" of cubanes. The following properties will be discussed: Orientational ordering phase transitions take place at unusually low temperatures. The significant size and shape recognition makes possible the design of the crystal structure of new higher fullerenes and substituted cubane derivatives. In the C_{70} and C_{76} derivatives fullerenes precess about the same crystallographic axis, establishing the basis of future molecular motors. At elevated temperatures the decomposition of cubane induces topochemical copolymerization with the surrounding fullerenes. Polymerized single crystals preserve their macroscopic crystalline character with shiny flat surfaces up to the decomposition at 700 K.

Twenty International Winterschools in Kirchberg: How come?

20:10 CEL 1

M. Mehring
Universität Stuttgart, Germany

You may wonder how it all started and how it came about to be continued for such a long time. Some of you were there right at the beginning and some of you are still here. This lecture will highlight some of the events and the scientific evolution of the International Winterschool in Kirchberg.

Nano-carbon materials: formation, characterization, and applications

20:50 CEL 2

Sumio Iijima
Research Center for Advanced Carbon Materials at AIST (also Meijo University and NEC)

15 years have passed since the discovery of carbon nanotubes and important physics of the materials has considerably progressed. Some of detailed comparison between experiment and theory however remains yet to be explored by using well-controlled specimens. Some of problems with obtaining well-controlled structure of nanotubes (diameter, length, quantity, chirality, structural perfection, impurity, homogeneity) seem to be overcome to some extent recently in our laboratories. Here a method of controlling tubule diameter of nanotubes will be presented in terms of optical spectroscopy. Another break-through in nanotube growth is the "Super-Growth" of single wall carbon nanotubes whose further development will be presented in this symposium by Hata (1).

In nanoscience and nanotechnology characterization of nano-structured materials is a substantial part of research. We have been emphasizing an importance of electron microscopy and challenged how far we can extend its technique to know local atomic structures and elemental analysis on individual atom basis. Here I would like to illustrate some of works that we have done so far including a historical background. One of current issues here is to know interaction between nanotubes and dopants that have been incorporated into nano-spaces of the nanotubes. Suenaga will introduce more recent development along this line in this symposium (2).

Last topic that I would like to present is a bio-medical application of the carbon nano-horns (CNHs). We utilize the large surface area of the CNHs comparable to activated carbon with emphasis on their chemical and physical stability due to pure graphitic structure. After studying gas adsorption properties of CNHs for some years, recently we have targeted on a drug carrier for the use of CNHs in drug delivery system. Loading and release of a drug on/from CNHs were studied in some quantitative manners and the loaded drugs were tested on living cells (3).

(1) T. Saito, et al., J. Phys. Chem. B, 109, 10647-10652 (2005). D. Futaba et al., Science 306, 1362-1364 (2004). D. Futaba et al., P.R.L 95, 056104 (1)-(4) (2005).

(2) A. Hashimoto, et al., Nature, 430, 870-873 (2004). K. Urita, et al., P.R.L, 94, 155502(2005). Z. Liu, et al., P.R.L., 95, 187406(1)-(4) (2005)

(3) T. Murakami et al. Mol. Pharm. (2004). K. Ajima, et al., Mol. Pharm., 2, 475-480 (2005). K. Shiba, et al., Small, 1, 1180-1183 (2005).

Theory

8:30 – 9:00 **M. MACHON, D**
Electron phonon coupling in carbon nanotubes

9:00 – 9:30 **A.C. FERRARI, UK**
Electron phonon coupling, Raman spectra and electron transport in nanotubes

9:30 – 10:00 **F. MAURI, F**
Hot phonons in carbon nanotubes and superconductivity in Ca intercalated graphite

10:00 – 10:30 **Coffee break**

10:30 – 11:00 **S. SAITO, JP**
Superconductivity in carbon: from C_{60} *to diamond*

COMMERCIALS

11:00 – 11:30 **S. REICH, US**
Chirality control of carbon nanotubes by epitaxial growth

11:30 – 12:00 **J.M. CARLSSON, D**
Structural and electronic properties of vacancies in nanotubes

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

Application, chemistry

18:30 – 19:00 **R. SCHLÖGL, D**
Surface chemistry and heterogeneous catalysis of carbon nanostructures

19:00 – 19:30 **A. HIRSCH, D**
Chemical functionalization of fullerenes and carbon nanotubes

19:30 – 20:00 **N. WONG SHI KAM, US**
Exploiting the intrinsic properties of single-walled carbon nanotubes for transport and delivery of biological cargos and triggering cell death

Poster II (M–Z)

8:30
THEO 1

Electron phonon coupling in carbon nanotubes

M. Machon, S. Reich, and C. Thomsen
Technische Universität Berlin, Germany; Massachusetts Institute of Technology, Cambridge, USA

Knowledge of electron-phonon coupling is essential for the understanding of many properties of carbon nanotubes. Ab initio calculations of the electron-radial-breathing-mode coupling predicted a radius, chirality, and family dependence which could explain the intensity patterns found in Raman experiments [1,2].

We review these results and present electron-phonon calculations for the totally symmetric high-energy mode(s) of nanotubes. The coupling of the high-energy mode is stronger than for the radial breathing mode and shows similar chirality and family dependencies. We do not find a direct diameter dependence except for very small-diameter nanotubes, which show a specially strong coupling.

We further present UV-Raman measurements of nanotubes grown in zeolite. In the UV range we access the (3,3) nanotube and show evidence for its predicted strong electron-phonon coupling and their giant phonon softening [3,4].

[1] H. Telg et al., Phys. Rev. Lett. 93, 177401 (2004).
[2] M. Machon et al., Phys. Rev. B 71, 035416 (2005).
[3] K.-P. Bohnen et al., Phys. Rev. Lett. 93, 245501 (2004).
[4] D. Connetable et al., Phys. Rev. Lett. 94, 015503 (2005).

9:00
THEO 2

Electron phonon coupling, Raman spectra and electron transport in nanotubes

A.C. Ferrari[1], S. Piscanec[1], M. Lazzeri[2], J. Robertson[1], and F. Mauri[2]
[1] Cambridge University, Engineering Department, Cambridge, UK
[2] Institut de Mineralogie et Physique des Milieux Condenses, Paris, France

Electron-phonon coupling (EPC) is a key physical parameter in carbon nanotubes. Here we discuss its effects on optical phonon dispersions, Raman spectra and electron transport. The main effect on phonons is the onset of Kohn anomalies (KA). These are distinct features in metallic systems, associated to the presence of a Fermi surface [1]. Graphite has two KA for the Gamma-E2g and K-A?1 optical modes [2], resulting in two sharp kinks. Due to the reduced dimensionality, KA are enhanced in metallic tubes, but absent in semi-conducting [2,3]. We show that EPC is the major source of broadening for the Raman G and G- peaks in graphite and metallic tubes [3,4]. We assign the G+ and G- peaks to TO (circumferential) and LO (axial) modes. We then present five independent approaches to directly measure the optical phonons EPC in graphite and nanotubes from their phonon dispersions and Raman spectra. These measurements allow us to quantify the EPC effects on high field electron transport in nanotubes. High field measurements show that electron scattering by optical phonons breaks the ballistic behaviour [5]. We derive a simple formula for the electron mean free path for optical phonon scattering in high-field transport [6]. Comparison with the experimental scattering lengths [5] shows that hot phonons are created during high-bias transport [6]. Their effective temperature can be thousands K and sets the ultimate limit of ballistic transport [6].

1. W. Kohn, Phys. Rev. Lett. 2, 393 (1959).
2. S. Piscanec et al. Phys. Rev. Lett. 93, 185503 (2004).
3. S. Piscanec et al. Phys. Rev. B submitted (2005).
4. M. Lazzeri et al. cond-mat/0508700.
5. Z. Yao et al. Phys. Rev. Lett. 84, 2941 (2000).
6. M. Lazzeri et al. Phys. Rev. Lett. 95, 236802 (2005).

Hot phonons in carbon nanotubes and superconductivity in Ca intercalated graphite

9:30 THEO 3

F. Mauri, M. Calandra, and M. Lazzeri
Universite Pierre et Marie Curie

Electron-phonon interaction rules many peculiar behaviors of graphite-based materials. I will present two remarkable examples (i) the generation of hot phonons in carbon nanotubes (CNT) by electron transport and (ii) the superconductivity of Ca intercalated graphite.
In the first part, I will demonstrate the key role of phonon occupation in limiting the high-field ballistic transport in metallic CNT [1]. To this purpose, we solve the coupled Boltzmann transport equations for both electrons and phonons. We faithfully reproduce the measured IV curves and we find a phonon effective temperature of several thousands K (hot phonons). This suggests that we can improve the performances of CNT as interconnects, by reducing the hot-phonon temperature.
In the second part, I will study the origin of superconductivity in intercalated graphite (IG). Alkali IGs are known to superconduct with a critical temperatures (Tc) of the order of the K. At the IWEPNM05, we learned with surprise that Ca IG (CaC6) is a superconductor with the sizable Tc of 11.5 K [2,3]. Using density functional theory I will demonstrate that superconductivity in C6Ca is phonon-mediated [4] and mostly due to C vibrations perpendicular and Ca vibrations parallel to the graphite layers. A non zero electron-phonon coupling for these modes can not be associated the Fermi surface of the graphite pi bands but requires the presence of a second Fermi surface associated to the intercalant atoms. This result suggests a general mechanism for the occurrence of superconductivity in IG: superconductivity requires an intercalant Fermi surface since the simple doping of the pi bands in graphite does not lead to a sizable electron-phonon coupling. This condition occurs if the intercalant band is partially occupied, i. e. when the intercalant is not fully ionized.

[1] M. Lazzeri, F. Mauri, preprint available on demand.
[2] Weller et al, Nature Physics 1, 39 (2005).
[3] Emery et al, Phys. Rev. Lett. 95, 087003 (2005).
[4] M. Calandra, F. Mauri, Phys. Rev. Lett. 95, 237002 (2005).

Superconductivity in carbon: from C_{60} to diamond

10:30 THEO 4

Susumu Saito, Tomohisa Maeda, and Takashi Miyake Tokyo Institute of Technology, JP

For many years it has been a grand dream to dope holes into solid C_{60}. The large Fermi-level density of states in alkali-doped C_{60} superconductors is one of the main reasons for their high transition temperatures. Hole doping into solid C_{60} would give rise to also large Fermi-level density of stats. Previously we showed that the substitutional B doping would be the most plausible way of hole doping. In this context, a recent discovery of superconductivity in B-doped diamond is of high interest and importance. Its transition temperature has reached 11 K in the heavily B-doped thin film grown on the (111) surface. We have studied the electronic structure of heavily B-doped diamond in the framework of the density functional theory. Interestingly the "(111)" film is found to have several distinct advantages over the "(100)" film. In addition, based on the GW study, we point out the importance of the band-gap reduction in considering the electronic structure of doped metallic diamond.

Chirality control of carbon nanotubes by epitaxial growth

11:00 THEO 5

S. Reich[1], L. Li[1], and J. Robertson[2]
[1] Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, US
[2] Department of Engineering, University of Cambridge, 9 JJ Tompson Avenue, Cambridge CB3 0FA, UK

We propose an idea for the chirality-selective growth of single-walled carbon nanotubes based on two key concepts: Chiral selectivity can be achieved by controlling the carbon cap that nucleates on the catalyst particle. Once a cap is finished, it grows into a unique nanotube. We suggest that specific caps (and hence tubes) can be selected by epitaxial growth on a solid catalyst. Lattice matched caps are by $0.1 eV/C$ more stable on a Ni surface than non-lattice matched structures. Our first-principles calculations of the formation energy of small-diameter nanotube caps on Ni excellently explain the dominance of certain chiralities in low-temperature chemical vapor deposition.

11:30
THEO 6

Structural and electronic properties of vacancies in nanotubes

Johan M. Carlsson and Matthias Scheffler
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Perfect nanotubes have extraordinary properties, but real nanotubes contain defects and impurities. This may have a noticeable effect on strenght, conductivity, and chemical properties. We have therefore studied how curvature and vacancies change the local structure of nanotubes and how this in turn influences the electronic properties.

Our density-functional theory (DFT) calculations show that atomic relaxations at vacancies rebind undercoordinated atoms such that a combination of non-hexagonal rings is formed. This leads to buckling and a local contraction of the radius in nanotubes. The vacancies tend to align along the tube axis and the formation energy diminishes in the smaller tubes when the curvature increases.

The presence of the vacancies perturbs the pi-band such that a defect state appears close to the Fermi level. Such defect states can lead to local charging and contribute to an increased chemical activity. The curvature in nanotubes mixes the defect states with the pi-band such that the chemical properties will depend on the radius of the nanotube.

FutureCarbon GmbH

Company Profile

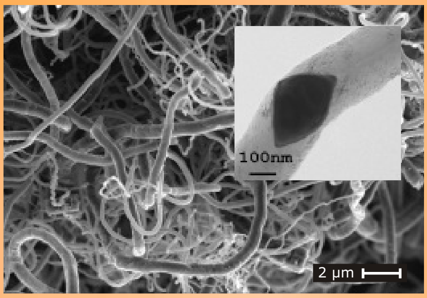
FutureCarbon develops and produces carbon-nanomaterials. In July 2002 FutureCarbon was founded as an affiliated company of FutureCamp GmbH. Our experience and technical background emanate from the vast know-how of the former Mannesmann Pilotentwicklung. We are located in Bayreuth in the newly build Center of Excellence New Materials. This site and the close vicinity of the University of Bayreuth with its faculty of applied natural sciences offer excellent working conditions. The materials are produced in a computer controlled CVD-apparatus and are extensively characterised afterwards. We provide scanning and tunneling electron microscopy and BET and further methods as contracted with the customer. Our goal is to fully satisfy our customers wishes. Therefore we individually select the appropriate type of fiber as well as the chemical modifications to adopt our products to our customers specific applications.

CNF-HB CarbonNanoFibers Herringbone

Diameter:	200 - 600 nm
Length:	5 - 50 µm
Purity:	95 % (raw) 99 % (purified)
BET:	ca. 60 m²/g

Properties:
Enhanced mechanical strength, rheological and tribological properties

Applications:
Elastic foams, Composites
Dielectricity, Batteries, Carbon mats and paper, Flame retardance

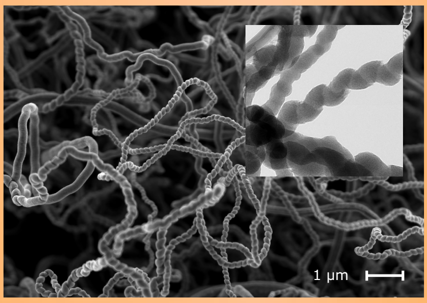


CNF-SC CarbonNanoFibers Screws

Diameter:	50 - 200 nm
Length:	1 - 10 µm
Purity:	90 % (raw) 99 % (purified)
BET:	ca. 150 m²/g
Ratio `Screws' type in product:	about 75 %

Properties:
Enhanced mechanical strength and ductility

Applications:
Foams and porous networks
Composites, Gas adsorption

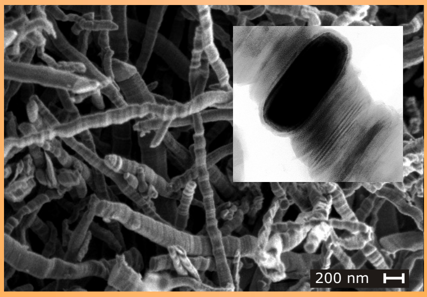


CNF-PL, CarbonNanoFibers Platelet

Diameter:	100 - 250 nm
Length:	0,5 - 5 µ
Purity:	95 % (raw) 99 % (purified)
BET:	ca. 100 m²/g

Properties:
Electrical conductivity, wettability, Enhanced rheological and tribological properties

Applications:
Catalyst support, Composites

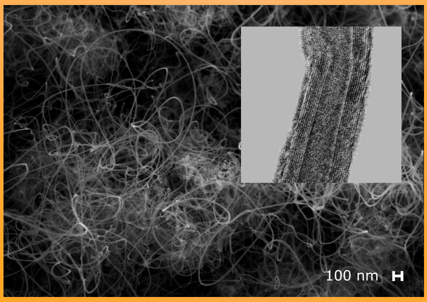


CNT-MW, CarbonNanoTubes Multiwalled

	Quality I	Quality II
Diameter:	10 - 20 nm	20 - 50 nm
Length:	5- 50 µm	5 - 50 µm
Purity:	95 % (raw) 99 % (purified)	95 % (raw) 99 % (purified)
BET:	ca. 200 m²/g	ca. 200 m²/g

Properties:
Enhanced mechanical strength, electrical and thermal conductivity, rheological and tribological properties

Applications:
Composites: polymers, resins, glas, ceramics etc.
Soil-resisting and hydrophobic surfaces,
Catalyst support
Foams, Gasadsorption
Flame retardance



Pictures: Clarissa Abetz

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Surface chemistry and heterogeneous catalysis of carbon nanostructures

18:30 APPLc 1

Robert Schlögl
Fritz-Haber-Institut der MPG, www.fhi-berlin.mpg.de

Carbon nanostructures are frequently studied for their unusual physical properties giving rise to a wealth of phenomena and potential applications centred on their nanoscopic dimensions.

These dimensions give also rise to particular chemical reactivity characterised by a combination of graphitic (metallic) transport properties and poly-olefinic localized organic functional group chemistry. This ideal chemistry is strongly modified by local defect chemistry augmenting the variability of organic functional groups, in particular with oxygen and hydroxyl groups stemming from the reaction with ambient air.

The contribution briefly reviews the analytics of these properties with spectroscopic and chemical methods. It then reviews the potential of carbon nanostructures in heterogeneous catalysis. The dual functionality of metallic and solid acidic (from local functionalisation) allows for developing metal-free catalysts for selective oxidation, hydrogenation and dehydrogenation.

Chemical functionalization of fullerenes and carbon nanotubes

19:00 APPLc 2

Andreas Hirsch
Institut für Organische Chemie, Universität Erlangen-Nürnberg

The core surface of C_{60} provides an ideal platform for the attachment of functional addends in a globular arrangement. The defined addition of a selected combination of functional groups at specific sites of the fullerene framework allows for the synthesis of new molecular architectures with unprecedented properties. For this purpose the complete control over the regioselectivity of subsequent additions to the [6,6]-bonds of the C_{60} framework is an important requirement. We achieved this goal by the introduction of new functionalization concepts. One strategy takes advantage of the even distribution of strain within flexible macrocyclic malonate addends. Based on these synthetic methods the tailor design of a large variety of functional fullerene derivatives with properties such as photo-induced charge separation, liposome formation and biological activity was possible. Typical examples are pi-stacked dyads and the first globular lipids. The chemical functionalization of carbon nanotubes opens up a variety of opportunities. First – the attachment of suitable organic or polymeric groups increases the solubility in water or in organic solvents and allows for individualization and further characterization of the tubes. Second – an increase in solubility is accompanied by an increase of processability, such as the improved incorporation in polymer matrices. Third – the unique properties of the carbon nanotube can be combined with those of other functional materials. Fourth – chemical functionalization might be the key point for the separation of metallic from semiconducting tubes by taking advantage of different reactivities. In this contribution we report on several methods for the chemical functionalization of single- and multi walled carbon nanotubes. Examples are side wall additions of a reactive species such as nitrenes, carbenes, radicals and nucleophiles and defect functionalization of pre-existing attachments such as carboxylic groups. Next to the chemical modification itself the physical and spectroscopic properties of the functionalized tubes as well as new concepts for their incorporation into polymer matrixes is reported.

Exploiting the intrinsic properties of single-walled carbon nanotubes for transport and delivery of biological cargos and triggering cell death

19:30 APPLc 3

Nadine Wong Shi Kam and Hongjie Dai
Department of Chemistry, Stanford University

The application of single-walled carbon nanotubes (SWNT) for breaching the cellular membrane to transport and deliver biological cargoes is reported. The SWNTs cellular internalization pathway is determined to be a clathrin-dependent endocytosis. Functionalization schemes are also developed to incorporate cleavable bonds and load multiple cargos on the nanotube transporter. The SWNT transporters have no apparent cytotoxic effects or detrimental effect on biological functionality of the cargo post-internalization. The intrinsic optical properties of SWNT are exploited to cause local heating into cell and can be combined with targeting molecules to trigger cell death selectively in cancer cells. SWNT are emerging as a new class of cellular transporters for applications in drug delivery, protein delivery, gene therapy and cancer therapy. Preliminary studies are currently under way to assess the biocompatibility of SWNT and their delivery ability in-vivo.

CYTOTOXICITY OF CARBON BASED NANOMATERIALS

PTh 1

A. Magrez[1], S. Kasas[1,2], V. Salicio[3], N. Pasquier[4], J.W. Seo[1], M. Celio[3], S. Catsicas[1], B. Schwaller[3], and L. Forró[1]
[1]EPF Lausanne, Switzerland. [2]Uni Lausanne, Switzerland. [3]University of Fribourg, Switzerland. [4]Laboratory Cytopath, Carouge Switzerland

The professional and public exposure to carbon based nanomaterials (CBNS) is supposed to dramatically increase in the coming years. Thus, it is primordial to know the health hazards related to their exposure. We performed studies on cultured cells exposed to three different types of CBNs: carbon nanotubes (MWCNTs), carbon fibers (CNFs), and carbon nanoparticles. Severe inhibition of cell proliferation and cell death have been observed, which become more pronounced as the aspect ratio of CBNs decreases and with the presence of chemically active functional groups on the graphene surfaces. These results indicate that more attention has to be paid to the health concerns of CBNs before pushing their application forward.

EFFECTS OF INTERMOLECULAR INTERACTIONS AND LATERAL HYDROGEN BONDING IN OLIGO(ETHYLENE GLYCOL) CONTAINING SELF-ASSEMBLIES

PTh 2

Lyuba Malysheva, Alexander Onipko, and Bo Liedberg
Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine; Division of Molecular Physics, Department of Physics, Chemistry and Biology, Linköping University,

Effects of intermolecular interactions including lateral hydrogen bonding are crucial in determining properties of self-assemblies of oligo(ethylene glycol) (OEG)-terminated alkanethiolates on gold. In this study, we consider the interplay between intra- and intermolecular interactions within OEG-terminated self-assembled monolayers (SAMs) by combining ab initio and molecular mechanics (MM) methods. Using our previous results from ab initio modeling of molecular geometry and vibrational spectrum of the OEG-SAM constituents (the approach has been shown to be very efficient for the consistent interpretation of infrared reflection-absorption spectra, Malysheva et al., JPC A 2005, 109, 7788), we performed MM modeling of OEG-terminated and amide group containing SAMs on gold. The most stable structures with the OEG terminus in either the all-trans or helical conformation are identified, and the range of variation of tilt, rotation and azimuthal angles, determining the orientation of molecules within the respective SAMs, are thoroughly discussed. We also report an improved understanding of the influence of lateral hydrogen bond formation on the conformational stability of OEG-containing SAMs.

A monopole-dipole model to compute the polarization properties of carbon nanotubes

PTh 3

Alexandre Mayer, and Philippe Lambin
Facultés Universitaires Notre-Dame de la Paix

In order to compute the polarization properties of carbon nanotubes, we developed a model in which each atom is described by both a net electric charge and a dipole. Compared to dipole-only models, the consideration of net electric charges enables one to address the fact that electrons move from one part of the nanotube to the other in response to an external field. It also enables one to account for the accumulation of extra charges, which is essential for the modelling of field emission. [1,2]

In a second part of this work, we combine this atomistic description of the nanotubes with a dielectric-function representation of its environment. This environment may consist of protrusions of the metallic substrate, nearby electrodes used for the focussing of the emission beam, and even water in a dielectrophoresis experiment. This extended technique then provides the nanotube polarization, the charge transfers as well as the relevant electric forces. [3]

Finally, in order to address dynamic aspects in the polarization of nanotubes, we account for the frequency-dependence of the atomic polarizabilities. This enables one to generalize the previous results to situations in which the external field is oscillating. [4]

[1] A. Mayer, Phys. Rev. B 71, 235333 (2005).
[2] A. Mayer, Appl. Phys. Lett. 86, 153110 (2005).
[3] A. Mayer and Ph. Lambin, Nanotechnology 16, 2685 (2005).
[4] For additional references, please visit `http://www.fundp.ac.be/~amayer`

PTh 4

MICROWAVE EXPERIMENTS AND DOUBLE QUANTUM DOTS IN CARBON NANOTUBES

C. Meyer[2], S. Sapmaz[1], P. Jarillo-Herrero[1], P. Beliczynski[1], and L.P. Kouwenhoven[1]
[1]Kavli Institute of Nanoscience, Delft University of Technology; [2]Research Centre Jülich, Institute of Solid State Research

Single-walled carbon nanotubes (SWCNTs) are one-dimensional conductors, either metallic or semiconducting depending on their chirality. In the past years, the study of quantum transport through SWCNTs has revealed many quantum phenomena, e.g. quantum dot shell filling, Fabry-Perot-like interference, Kondo effect, etc.

Here, we show first experiments, in which a single quantum dot on a nanotube is irradiated with microwaves. This leads to photon assisted tunneling which can be used for spectroscopy. In contrast to similar experiments done in GaAs structures, we observe not only spin but also orbital excited states. If one assumes the tunnel barriers of the contacts to be equal, this method gives a lower bound for the orbital relaxation time of 45 ns. However, to verify this one needs control over the tunnel barriers.

As second step, we show that we can fabricate gate structures that allow us to introduce and control tunnel barriers by using narrow top-gates. Such, we can form double quantum dots (QDQ) and tune the coupling between the two dots. We observe shell filling and excited states in the QDQ.

In combination, these experiments open up the opportunity for a scalable electron spin quantum computing concept, if microwaves can be coupled to the system.

PTh 5

Dynamics of a Fullerene Quantum Gyroscope

K.H. Michel, and B. Verberck
Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

Raman scattering experiments on solid endohedral fullerene C2Sc2@C84 reveal the quantized rotational motion of a diatomic C2 unit as a plane molecular rotor [1]. We present a theoretical description of the composite dynamics of a C2 planar rotor inside the moving Sc2C84 cage. While the dynamics of the C2 rotor is treated by quantum mechanics, the dynamics of the cage is treated by classical mechanics including reorientations and librations. Time dependent correlation functions are calculated. The convolution of the classical and quantum mechanical motion leads to a line broadening of the plane quantum rotor energy levels measured by Raman scattering.

[1] M. Krause, M. Hulman, H. Kuzmany, O. Dubay, G. Kresse, K. Vietze, G. Seifert, C. Wang, and H. Shinohara, Phys. Rev. Lett. 93, 137403 (2004).

PTh 6

EFFECT OF ULTRAVIOLET IRRADIATION ON ALIGNED CARBON NANOTUBE FIBERS

C. Mikó, J.W. Seo, R. Gaál, A. Kulik, and L. Forró
Ecole Polytechn. Fed. Lausanne, CH

In order to exploit the exceptionally high mechanical properties of carbon nanotubes (CNTs), one of the major challenges is the processing of CNTs on macroscopic scale, for instance into oriented single-walled carbon nanotube (SWNT) fibers. Unfortunately SWNTs preferentially form bundles, where tubes interact via van der Waals force, and therefore the mechanical strength of these fibers are mainly dominated by the shear modulus.

Recently, we have demonstrated that electron irradiation can create cross-linked CNTs within SWNT ropes resulting in an increased Young's modulus. However, increasing dose leads to deterioration of the CNT wall structure and a significant loss of both mechanical strength and electric conductivity. Therefore an alternative non-destructive way is desirable to strengthen the fibers.

CNT fibers were irradiated by ultraviolet (UV) light. In-situ resistivity and mechanical measurements revealed that illumination by UV light leads to cross-linked nanotubes in the fiber, which can be explained by the photo-chemistry between the functional groups on the surface of CNTs and DMF molecules are trapped between the nanotubes. Both the conductivity and the mechanical strength significantly increase upon illumination leaving the graphitic structures intact, which makes UV irradiation more promising for reinforcement of CNT fibers.

Magnetic Properties of Carbon Nanofoam

PTh 7

D. Arèon, P. Cevc, Z. Jagličič, A. Zorko, T. Apih, F. Milia, and R. Blinc
J.Stefan Institute, University of Ljubljana

Ferromagnetism is typically the property of transition metals where there are unpaired electrons in unfilled atomic shells even in the solid. Nevertheless various form of carbon show ferromagnetic or ferromagnetic-like behaviour such as the purely organic ferromagnet TDAE-C_{60} [1], polymerized C_{60} forms [2], hydrogenated amorphous carbon [3] and cluster assembled carbon nanoform [4]. This system which has an ultra-low density (2-10 mg/cm3) is obtained by laser ablation of glassy carbon in an argon atmosphere [4, 5]. In carbon nanofoam a large difference between field cooled (FC) and zero field cooled (ZFC) magnetic susceptibility has been observed (5). Some samples show a maximum in the magnetic susceptibility between 50 K and 100 K characteristic of spin-glasses. A weak ferromagnetic like hysteresis curve has been observed at 2 K between 5 T and - 5 T with a saturation magnetization of MS 0.3 emu/g. Proton NMR measurements on absorbed water at room temperature showed the existence of two components in the magnetization decay. One has a T1 of about 0.8 msec and the other of about 200 msec. This demonstrates the inhomogeneous nature of the magnetization in carbon nanofoam with magnetic island embedded in a non-magnetic medium. Similar results are also obtained by EPR where three different well separated magnetic centers with different T1 values have been observed.

NOVEL ROUTE TO (BIO)-POLYMER NANOTUBE COMPOSITES

PTh 8

A.I. Minett[1], J.N. Coleman[2], M. Panhuis[3], W.J. Blau[2], and G.G. Wallace[1]
[1] ARC Centre for Electromaterials Science, Intelligent Polymer Research Institute, University of Wollongong, NSW 2522, Australia. [2] Department of Physics, Trinity College Dublin, Dublin 2, Ireland. [3] Department of Chemistry, The University of Hull, Hull, HU6 7RX, United Kingdom.

Novel polymer nanotube composites were fabricated by intercalating either polyvinylpyrrolidone (PVP) as a reference material and various biopolymers into carbon nanotube architectures from solution. This was carried out for both low (10k g/mol) and very high (1.3M g/mol) molecular weight polymers into buckypaper, fibres or stand-alone forests. Measurements of the polymer mass uptake as a function of time allowed the calculation of diffusion co-efficients for the various polymer and biopolymer strands respectively. Comparison of these co-efficients suggests that each polymer type undergoes a different mode of diffusion: normal diffusion for the low molecular weight polymers, but reptation for the high molecular weight polymers. This means that while the low weight polymer retains its randomly coiled conformation during diffusion and adsorption, the high weight polymer is forced to adopt an extended, high entropy state. These differences are reflected in the mechanical properties of the intercalated architectures. While reinforcement was observed in all cases, modulus (increase up to ≈3.5x) and strength (≈6x) enhancement were more efficient for the longer chain polymers. However the architectures intercalated with the shorter chain molecules were much tougher (≈25x). This novel route to tailored mechanical properties could be expected to be applied to any nanomaterial composite.

PHOTOLUMINESCENCE MAPPING OF VARIOUS (N, M) NANOTUBES BY CROSS-POLARIZED ABSORPTION

PTh 9

Yuhei Miyauchi, Mototeru Oba, and Shigeo Maruyama
Dept. of Mech. Eng., The Univ. of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Photoluminescence excitation (PLE) spectroscopy of single-walled carbon nanotubes (SWNTs) have been extensively studied for characterization of their unique electronic properties. In this report, we have studied polarized PLE spectra of various (n, m) nanotubes in surfactant suspension. Using a simple theory for PL anisotropy, we have obtained decomposed-PL maps for parallel and perpendicular polarization from two PL maps measured by so-called L-format method [1]. For some (n, m) nanotubes, distinct peak splitting of E12 and E21 transitions for perpendicular polarization was observed. Average of observed E12 and E21 energies was considerably larger than average of E11 and E22, although the average of E12 and E21 should give close agreement with that of E11 and E22 within tight-binding calculation of SWNT considering geometry optimization and curvature effect [2]. This qualitative discrepancy between measurement and calculation indicates the different amount of excitonic effect for each state. Detailed experimental techniques and results will be discussed.

[1] J.R. Lakowicz, Principles of Fluorescence Spectroscopy, Plenum Pub. Corp., New York, 1999. [2] M. Oba, S. Okada, T. Miyake, S. Maruyama, the 30th Fullerene Nanotubes General Symposium, Nagoya (2006).

PTh 10

Bang-bang control of fullerene qubits using ultrafast phase gates

John J.L. Morton[1][2], Alexei M. Tyryhskin[3], Arzhang Ardavan[2], Simon C. Benjamin[1], Kyriakos Porfyrakis[1], S.A. Lyon[3], and G. Andrew D. Briggs[2]
[1] Department of Materials, Unversity of Oxford; [2] Clarendon Laboratory, University of Oxford; [3] Dept. of Electrical Engineering, University of Princeton

Quantum information processing (QIP) harnesses the profound phenomena of quantum mechanics to manipulate information in radically new ways. A fundamental challenge in all QIP technologies is the corruption of superposition in a quantum bit (qubit) through interaction with its environment. Quantum bang-bang control provides a solution by repeatedly applying "kicks" to a qubit, thus disrupting an environmental interaction. However, the speed and precision required for the kick operations has presented an obstacle to experimental realization. Here we demonstrate a phase gate of unprecedented speed on a nuclear spin qubit in a fullerene molecule, N@C_{60}, and use it to bang-bang decouple the qubit from a strong environmental interaction. We can thus trap the qubit in closed cycles on the Bloch sphere, or lock it in a given state for an arbitrary period. Our procedure uses operations on a second qubit, a coupled electron spin, to generate an arbitrary phase on the nuclear qubit. We anticipate that the approach will be important for QIP technologies, especially at the molecular scale where other strategies, such as electrode switching, are unfeasible.

PTh 11

Controlled growth of metal-filled carbon nanotubes and their properties

C. Müller, S. Hampel, A. Leonhardt, D. Golberg, D. Elefant, H. Reuther, and B. Büchner
Carbon nanotube growth and selection

Multi-walled carbon nanotubes can be filled with various elements and compounds. Among these materials magnetic fillings have significant potential for new applications in electronic or biomedicine.
We show a CVD-route for the growth of metal-filled carbon nanotubes (Fe, Co, Ni) on pre-structured silicon and alumina substrates. The nanotube dimensions (length, diameter, filling) can be influenced by the nature of the catalyst on the substrate as well as by the process conditions. The filled nanotubes were obtained due to continuous decomposition of metal-containing precursors (e.g. metallocenes) in an Ar atmosphere at about 800°C. Beside the synthesis the multi-walled carbon nanotubes were investigated with x-ray diffraction (XRD), Mössbauer spectroscopy and transmission electron microscopy (TEM) to obtain further information about the composition, the crystal size and the crystal orientation of the metal-nanorods. In addition the magnetic properties of nanotube ensembles were studied and compared with theoretical data.

PTh 12

Carbon Nanotube Networks as Selective Hydrogen Sensors

Edgar Munoz[1], Isabel Sayago[2], Eva Terrado[1], Manuel Aleixandre[2], Maria del Carmen Horrillo[2], Maria Jesus Fernandez[2], Esperanza Lafuente[1], Wolfgang K. Maser[1], Ana M. Benito[1], Javier Gutierrez[2], and Maria Teresa Martinez[1]
[1] Instituto de Carboquímica (CSIC), 50018 Zaragoza, Spain; [2] Laboratorio de Sensores (IFA-CSIC), 28006 Madrid, Spain

Selective carbon nanotube-based hydrogen sensors were fabricated by simply airbrushing Pd-functionalized single-walled carbon nanotube (SWNT) dispersions on alumina substrates. The hydrogen sensing capabilities of the resulting thin films were evaluated by dc electrical measurements in nitrogen and air atmospheres. Pd-functionalization of the employed SWNTs enabled increasing the device sensitivity to hydrogen. The fabricated sensors exhibited good sensitivity and selectivity to hydrogen at room temperature in reversible and reproducible hydrogen detection processes. The response to hydrogen and the cross-sensitivity to gases such as ammonia, toluene and octane were studied. The effect of aging, thermal treatment and the employed carrier gases on the sensor performance were also investigated.

FABRICATION OF FIELD-EFFECT TRANSISTOR DEVICES WITH FULLERENE RELATED MATERIALS

PTh 13

Takayuki Nagano, Kenji Ochi, Haruka Kusai, Hiroyuki Sugiyama, Kumiko Imai, Yoshihiro Kubozono, and Akihiko Fujiwara
Okayama Univ., JST-CREST, JAIST

Field-effect transistor (FET) devices with organic thin films have many advantages such as large-area coverage, structural flexibility, portability, and shock-resistance. The SiO2 gate insulators in organic FET devices have been replaced by polymer gate insulators in order to bring out these advantages during past years. In this study, we have first fabricated flexible fullerene FET devices with various types of polymer gate insulators on the poly(ethylene terephthalate) (PET) substrates. The n-channel normally-off FET properties were observed in the C_{60} FET device with polyimide gate insulator. The field-effect mobility was determined to be ≈10-2 cm2 V-1 s-1 at 300 K. On the other hand, the n-channel normally-on FET properties were observed in the solution-processed fullerodendron FET device with polyvinyl alcohol (PVA) insulator. Moreover, we have fabricated FET devices with thin films of higher fullerenes and endohedral metallofullerenes in order to search for suitable electronic materials for high performance FETs. All FET devices with thin films of fullerenes showed n-channel normally-on FET properties, which originated from high bulk currents due to small band gap energies of these materials. Thus, the FET properties in fullerene FET devices reflect directly intrinsic nature of fullerenes.

AHARONOV-BOHM EFFECTS ON CONDUCTIVITY IN CARBON NANOTUBES: AN INVESTIGATION OF STRAINS OR CURVATURE EFFECTS

PTh 14

T. Nakanishi and T. Ando
AIST, ISSP, CREST, and Tokyo Inst. Tech.

The Boltzmann conductivity is calculated for carbon nanotubes in the presence of an Aharonov-Bohm magnetic flux with taking into impurity and electron-phonon scatterings.[1] We show that effects of strains or curvature manifest themselves as a prominent conductivity peak as a function of the flux.
A small gap is induced in metallic carbon nanotubes by the strain or curvature effects, which is incorporated in the effective mass theory as an effective flux.
In the presence of magnetic flux the band gap diminishes and linear bands are restored, when the applied magnetic flux cancels with the effective flux.
A prominent peak appears in the calculated magneto-conductivity.
The appearance of the peak corresponds to the absence of backscattering in metallic linear bands.
The effective flux is so small that the peak can be observed easily using a conventional magnet.
Various information on the curvature and strain effects and a relative amount of short-range scatterers can be obtained by careful measurement of the conductivity in the presence of the magnetic flux and by changing the electron density through a gate voltage.
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AN ESSENTIAL ROLE OF CO2 AND H2O DURING AEROSOL (FLOATING CATALYST) CVD SYNTHESIS OF CNTS FROM CARBON MONOXIDE

PTh 15

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Single-walled CNTs were synthesized from CO and Fe catalyst nanoparticles by two different aerosol methods. Iron catalyst particles were produced either by a hot wire generator (HWG) method using a resistively heated iron wire or by thermal decomposition of ferrocene vapor. An essential role of etching agents (CO2 and H2O) for CNT formation in these methods was demonstrated. No CNTs were produced under clean wall reactor conditions, i.e. in the absence of CO2. The addition of small amounts of CO2 or H2O vapor in the reactor resulted in an increase in the CNT bundle as well as individual nanotube lengths. It was found that the CO2 concentration ranges at which CNTs can be produced are varied from 80 to 1500 ppm in the HWG setup and from 600 to 8000 ppm in the ferrocene setup. The introduction of 1000 ppm CO2 decreased the minimum temperature of CNTs synthesis to below 600°C. The function of CO2 and H2O is believed to be to etch amorphous carbon that can poison catalyst particles needed for CO disproportionation as well as for CNT nucleation and growth. The mechanism of CNT formation is discussed.

PTh 16

Contact dependence of carrier injection in carbon nanotubes: An ab initio study

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We combine ab initio density functional theory with transport calculations to provide a microscopic basis for distinguishing between 'good' and 'poor' metal contacts to nanotubes. Comparing Ti and Pd as examples of different contact metals, we trace back the observed superiority of Pd to the nature of the metal-nanotube hybridization. based on large scale Landauer transport calculations, we suggest that the 'optimum' metal-nanotube contact combines a weak hybridization with a large contact length between the metal and the nanotube.

PTh 17

ELECTRICAL TRANSPORT PROPERTIES OF HOT WALL EPITAXIALLY GROWN PARA-SEXIPHENYL NANO-NEEDLES

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Hot wall epitaxy (HWE) is a well known technique for growing highly ordered thin films of C_{60} and para-sexyphenyl nano-needles [1]. Here we report on first studies of electrical transport properties of HWE grown nano-needles of para-sexiphenyl on crystalline substrates. The needles are well aligned in one direction with average needle length and width in the order of 30 micrometer and 100 nanometer, respectively. We investigated the electronic properties of these nano-needles in top-gate organic field-effect transistor geometry using organic dielectrics as gate insulators with various metal electrodes as source-drain contacts. A temperature independent charge carrier mobility and its photoresponse will also be discussed.

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PTh 18

POLYMER RING FORMATION BY ELECTRON/HOLE INJECTION FROM AN STM TIP INTO A C_{60} CLOSE-PACKED LAYER

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Scanning tunneling microscope (STM) is a powerful tool for nanoscale modification of various surfaces. For the surface of C_{60} close-packed layer, carrier (electron/hole) injection from an STM tip brings on polymerization of C_{60} molecules. Polymerization of C_{60} is hard to be achieved at single molecular precision because of a spatial spread of injected carriers. In this study, the carrier-spreading effect has been investigated by mapping polymerization of C_{60} molecules. Experimental procedure is as follows: An STM tip was placed on an injection point at a certain tip-sample distance (sample bias voltage: 2.0 V, tunneling current: 0.2 nA). In order to induce polymerization of C_{60}, carrier injection was performed by application of voltage pulses with durations of 30 s. Resulting distribution of polymerized C_{60} molecules showed a beautiful ring-shaped structure. The polymer ring of C_{60} suggests that slowing down of radially spreading carriers is indispensable for polymerization of C_{60}. Therefore, the polymer ring can be considered as a direct reflection of carrier propagation. In addition, both polymerization and depolymerization of C_{60} has been found to be induced by injection of both electrons and holes.

TRANSPORT AND TEM ON DYSPROSIUM METALLOFULLERENE PEAPODS

PTh 19

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Single-walled carbon nanotubes produced by the arc-discharge method using non-magnetic catalysts were filled with (Dy@C82) endohedral metallofullerenes. Transport measurements were performed on (Dy@C82)@SWNT metallofullerene peapod bundles and on the corresponding empty SWNTs in transistor configuration. After the transport investigations the substrates were partially etched away enabling us to take TEM images of the same bundles and tubes on which transport had been carried out before. This procedure gives information on whether the sample measured was a single tube or a bundle and on the degree of tube filling. Latest results from these combined transport and TEM investigations will be discussed.

THIN FILMS of INDIVIDUAL SINGLE-WALL CARBON NANOTUBES for NON-LINEAR OPTICAL APPLICATIONS

PTh 20

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Recently we have demonstrated a potential of aqueous suspensions of individual single-wall carbon nanotubes (SWNT) for applications in non-linear optics. They have been shown as the efficient universal ultrafast beam modulators in resonators of lasers with wavelengths 1.06-1.54 mkm [1,2]. To increase the SWNT potential for such applications we have developed the growth procedures for SWNT solid films. Two approaches have been used. First, a chemical vapor deposition of SWNT from ethanol vapor [3] onto transparent substrates has been developed. The films grown have been characterized in detail by the electron microscopy and the Raman scattering techniques. The typical SWNT Raman spectra have been registered for a variety of synthesis regimes. The catalyst crystal growth has been optimized. Second, we have succeeded in preparation of "SWNT-polymer" thin films. The working characteristics of both types of SWNT films and aqueous suspensions have been compared for the fiber and solid state lasers.

The work is supported by RFBR 04-02-17618 and by RAS Presidium programs.

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ION-ELECTRON EMISSION FROM CARBON NANOTUBE CATHODE

PTh 21

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We recorded the ion current occurred in the result of desorption of molecules from carbon nanotube surface in an electric field. A sawtooth voltage regulated the electric field with certain frequency of 0.01 - 5 Hz. The ion current and current-voltage characteristics of cathode were measured at a time. The correlations between the potential for ion current appearance and the electron emission threshold were established for different types of carbon nanotubes. To understand the experimental results in detail the quantum-chemical calculations on models were performed. Effect of electric field on the binding energy of various molecules adsorbed on the top and body of carbon nanotube was examined.

PTh 22

CALCULATION OF OPTICAL CONSTANTS FROM CARBON NANOTUBE TRANSMISSION SPECTRA

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Precise determination of absorption coefficients α in carbon nanotubes is crucial if we want to use optical data for purity determination. The common procedure (built into the software of most spectrometers) is to use the Lambert-Beer expression ($-\log T = \delta cl$) to calculate the extinction coefficient δ from the measured transmission. δ is, however, proportional to α only when reflection can be neglected. Discrepancies are small in the visible/UV range but increase toward the near infrared and become considerable in the far infrared, where metallic nanotubes absorb light.

To get proper absorption data in regions with considerable reflection one can use the Kramers-Kronig relations on the transmission data, taking into account the Fresnel equations at high frequency and the more strict calculation based on impedance matching of a thin metallic layer at low frequency. This method is strictly valid only in case of free-standing films, but not for the generally used sample-substrate configuration. The multilayer fit method uses the Drude-Lorentz model of the dielectric function and it takes into account multiple reflections at the sample-substrate interface.

We present several nanotube spectra, demonstrating the difference between the three methods, and the limits of applicability of the Lambert-Beer expression.

PTh 23

NANOCRYSTALLINE BUCKLING IN CARBON FIBERS

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Carbon fibers are composites consisting of planar graphene basic structural units, whereas composites using carbon nanotubis are based on tubelike structures. Therefore, carbon fibers themeselves can be seen as a model system to study the mechanical properties of carbon based nanocomposite materials.

Single carbon fibers were deformed in bending and position-resolved X-ray patterns were collected from the tension to the compression region with a synchrotron radiation nanobeam of 100 nm size of a waveguide structure. A strain redistribution with a shift of the neutral axis is observed as well as considerable buckling of the nanosized carbon crystallites in the compression region. This work enlights the difficulties in the application of nanocomposites if the basic structural units are not perfectly aligned.

PTh 24

Gas Adsorption on Carbon Nanotubes

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In previous work, we studied hydrogen adsorption on carbon nanotubes using ESR spectroscopy at a single pressure (135 kPa) and temperature (4 K). We found that for SWNTs, the ESR signal was quenched upon adsorption, and for MWNTs, the signal intensity increased dramatically. Beyond speculation we did not have an explanation for the latter effect, while the former was assigned to hydrogen occupying preferentially defect sites.

In this work, we present pressure and temperature dependent data on the same or similar samples which confirm our previous findings. For example, for one of the SWNT samples, we found a hydrogen saturation pressure of 400 torr at ambient temperature. We also present data on tubes where defects have been introduced by acid digestion, and data on other gases than hydrogen such as ammonia and NO.

ADAPTIVE ELECTRONIC ZONE FOLDING FOR DFT CALCULATIONS OF PHONONS AND TEMPERATURE DEPENDENT ELECTRON-PHONON COUPLING EFFECTS IN NANOTUBES OF ARBITRARY SIZE AND CHIRALITY

PTh 25

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Density Functional Perturbation Theory (DFPT) [1] is the most accurate ab-initio computational tool for the investigation of phonons and electron-phonon coupling. Experimentally, the most commonly studied carbon nanotubes (CNTs) have diameters from 0.7 nm up to 3-4 nm, with hundreds to thousands of atoms per unit cell. Furthermore, in order to properly describe CNT phonons in correspondence of Kohn anomalies and Peierls distortions, meshes with thousands of k points are needed for the Fermi surface integration [2,3]. This makes calculations of CNT phonons a major challenge within standard DFT. Thus, most DFT studies in literature focus either on extremely small tubes or, for bigger diameters, neglect the effects of the electronic smearing on the phonon frequencies, which often leads to inaccurate results. Here, we present a novel adaptive electronic zone folding method, which allows us to efficiently and precisely calculate, within DFPT, the complete temperature-dependent phonon-dispersions and electron-phonon coupling for CNTs of any diameter and chirality [3]. This approach allows us to drastically reduce the CPU time demand of standard DFT. We demonstrate the efficiency of our method by reporting the phonon dispersions, Kohn anomalies, and Peierls distortions in metallic nanotubes with diameters up to 3 nm and in a temperature range of 4 to 3000 K [3].

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SELF-ASSEMBLING PROPERTIES OF MOSIx NANOWIRES WITH DIFFERENT BIOLOGICAL MATERIALS DIFFERENT BIOLOGICAL MATERIALS

PTh 26

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In the last few years the interest in producing nano-devices for biomedical and electronic application using self-assembling properties of nano-bio-materials has significaly increased, motivated by the prospect of molecular nanobiosensors for medical applications. The key to the progress in this area is nanostructure self-assembly and connectivity. Here we present the fuctionalization of MoSIx nanowires with different biomaterials via gold-sulfur covalent bond. These nanowires are a new class of one-dimensional inorganic materials, easy synthesized and with interesting properties. We show that 5 nm gold nanoparticles suspended in water can reproducibly self-attach to MoSIx nanowire ends. AFM investigations were done to characterize the gold functionalized nanowires. The obtained yield was found to be up to 40%. Breaking force measurements were performed in order to confirm the covalent attachment between the gold nanoparticles and the nanowires. We studied also self-assembling properties of MoSIx nanowires with biological molecules. We succeed to immobilize two different types of proteins on gold MoSIx nanowires sistem: tyroglobuline, which is an iodinated and sulfated protein with high molecular mass and stefin B, a small protein of 11 KDa. Breaking force measurements were carried out also in this case.

The experiments demonstrate the existence of a remarkably simple functionalization route for self-assembling of nano-bio molecular devices and sensors. The investigation of electronic properties of such devices using STM/CAFM is presented as well.

PTh 27

A COMPREHENSIVE MESO-MECHANICAL THEORY OF TWISTED MWCNTS

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Individual MultiWall Carbon Nanotubes have been incorporated in various NanoElectroMechanical devices where they are subjected to twisting cycles, because they serve either as torsional oscillators [1,2] or as rotor bearings [3], when the outer walls are tore apart. Recently, a torsional pendulum based on a single-walled carbon nanotube has been fabricated [4]. In addition to getting rid of the intricacies of inter-wall interactions, such a device may have other definite advantages over MWCNT-based NEMs. However, understanding the elusive mechanisms of inter-wall coupling in cyclically twisted MWCNTs is worthwhile in itself, and could turn out to be useful in other applications, yet to be explored.

Overall, the experimental evidence collected so far is quite puzzling. We propose a continuum theory in which defect populations of different sort, when triggered by successive twisting cycles, evolve and interact with one another, progressing in either the circumferential or the inward direction. Primitive defects are thought to be created in the outer wall by the interaction of Cr atoms with the C lattice structure, because chromium is evaporated onto the nanotube when fabricating the device. We believe our model provides the simplest mesoscopic format able to cover all of the seemingly contradictory experimental facts reported in [1-3].

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PTh 28

SYMMETRY-ADAPTED TIGHT-BINDING CALCULATIONS OF THE PHONON DISPERSION AND THE RESONANT RAMAN INTENSITY OF THE TOTALLY SYMMETRIC PHONONS OF SINGLE-WALLED CARBON NANOTUBES

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The atomistic calculations of the physical properties of perfect single-walled carbon nanotubes based on the use of the translational symmetry of the nanotubes face increasing computational difficulties for most of the presently synthesized nanotubes with up to a few thousand atoms in the unit cell. This difficulty can be circumvented by use of the helical symmetry of the nanotubes and a two-atom unit cell. We present the results of symmetry-adapted tight-binding calculations of the phonon dispersion and resonant Raman intensity of the totally symmetric A1 phonons of several hundred nanotubes.

In particular, we show that 1) the frequencies and the resonant Raman intensity of the RBM and the G-band modes show radius and chirality dependence and family patterns, 2) the strong electron - A1(LO) phonon interactions in metallic nanotubes lead to Kohn anomalies of the phonon branches and to their softening at the zone-center, 3) the G-band consists of a subband due to A1(LO) phonons of semiconducting tubes centered at 1593 cm-1, a subband of A1(TO) phonons at 1570 cm-1, and a subband of A1(LO) phonons of metallic tubes at 1540 cm-1. The latter prediction confirms previous theoretical results but disagrees with the currently adopted assignment of the G-band features.

PTh 29

ELECTRONIC PROPERTIES OF K-INTERCALATED SINGLE-WALLED CARBON NANOTUBES AND C60-PEAPODS STUDIED BY HIGH ENERGY SPECTROSCOPY

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We present recent results on the potassium-intercalation of single-walled carbon nanotubes (SWCNT) and C60-peapods using x-ray absorption spectroscopy (XAS) and high-resolution photoemission spectroscopy. We analyze details of the competitive charge transfer to the C60 guests and the SWCNT hosts in the peapods compared to that to the SWCNT sample by probing the unoccupied electronic density of states. The results complement measurements of the doping dependence of the valence band electronic structure by photoemission spectroscopy and give further insight into the interplay of the electronic contributions from the two constituents upon doping as opposed to that of the individual compounds.

Work is supported by DFG PI440/1

Generation of ultra-fast laser pulses using nanotube mode-lockers

PTh 30

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Many key applications of carbon nanotubes (CNTs) in electronic devices require individual tubes with given chirality for their optimum performance. However, chirality control is not necessary if we want to exploit their electronic properties to build ultra-fast optoelectronic devices. Indeed, single wall carbon nanotubes are efficient saturable absorbers, i.e. they are pass-high filters for light, becoming transparent for sufficiently high incident power [1,2]. This makes them ideal components for a wide range of photonic systems, such as all-optical switches, pulse compressors, noise regenerative filters, etc. Here, we report a simple way to fabricate CNT-polymer films, combining polyvinyl alcohol or polycarbonate with CNT solutions. We show that these composites are promising passive mode-lockers [3]. Their absorption maximum can be easily tuned by using CNTs of different average diameter [3]. We use them to fabricate an ultra-fast (600 fs) erbium doped fibre laser. We demonstrate wide spectral tunability of the output laser pulse (from 1560 to 1530 nm), by adding a dispersion control element in the cavity [3]. Our simple wet chemistry fabrication process makes CNT based mode-lockers very cheap and easy to package. This renders them very competitive when compared to existing technology based on semiconductor saturable absorber mirrors, which are molecular beam epitaxy grown multiple quantum wells requiring expensive packaging [4].

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TRANSITORS FROM SWNT CROSS-JUNCTIONS

PTh 31

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Cross shaped areas on a Si/SiO2 substrate are functionalized by amine groups. These functional groups are more attractive to carbon nanotubes then the bare SiO2 surface. With this method nanotubes can be adsorbed on desired, predefined areas. In combination with molecular combing aligned nanotubes are adsorbed on the functionalized areas. In two successive steps two crossing nanotubes are adsorbed. These objects are contacted by palladium leads using electron beam lithography. Transport characteristics over the cross junction is investigated by applying a bias voltage to the palladium leads.

Also different insulating materials are deposited between the two adsorption steps between the nanotubes. Transistor characteristics of such devices are investigated by applying a gate potential to one of the crossing nanotubes. The results are discussed in terms of field effect transistor behaviour and charge induced geometrical changes of the tubes.

EFFECTS OF CHEMICAL TREATMENTS ON THE VIBRATIONAL PROPERTIES OF SINGLE-WALLED CARBON NANOTUBES: A COMBINED INFRARED/RAMAN SPECTROSCOPIC STUDY

PTh 32

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Raman and IR spectroscopy have been used to characterize chemically treated single-walled carbon nanotubes (SWNTs). Whereas Raman spectroscopy indicates changes in the skeletal structure of the SWNTs, IR spectroscopy provides information on the chemical structure of the surface defects. A detailed knowledge of the defect structures and hence their reactivity is of utmost importance for further applications (chemical reactions, dispersion, composites, etc). Arc-discharge SWNTs were subjected to various physicochemical treatments such as high-temperature vacuum annealing, and H2O2, HCl, or HNO3 under microwaves or reflux. The samples were then characterised by Raman and IR spectroscopy. A common problem in Raman micro-analysis of SWNTs is the spatial irreproducibility of the band intensities. A new sample preparation technique has been developed to overcome this problem. We show by IR that free carboxilic acid groups (-COOH) are not formed as readily as commonly assumed and alternative functional groups are discussed. Furthermore, we investigated the effect of chemical treatment on the dispersability of SWNTs in water. The degree of dispersion is determined by Raman spectroscopy.

PTh 33

Effect of phenyl rings in liquid crystal molecules on SWCNTs studied by Raman spectroscopy

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The self-organization of thermotropic liquid crystals (LCs) has proved to be able to influence the order of carbon nanotubes (CNTs) by imposing on the tubes the same orientational alignment as the liquid crystalline matrix. As the CNT surface-LC molecule interaction is a dominant mechanism in this transfer of order, it is expected to have a relevant influence on the efficiency of ordering and dispersion of the CNTs. How the LC molecules interact with carbon nanotubes depends strongly on their molecular structure. Here we present a Raman spectroscopy study of the effect of the adsorption of phenyl rings in the rigid core of LCs on SWCNTs, using three different single-component liquid crystalline hosts with cores varying from a fully aromatic biphenyl to a fully cycloaliphatic bycyclohexane. The role of phenyl rings is clearly revealed through a shift of the RBM modes of the SWCNTs dispersed in the fully aromatic LC, while no shift was detected in the LC without phenyl rings. The phenyl rings thus strengthen the LC-CNT interaction, thereby aiding the dispersion and ordering of SWCNTs, as confirmed by polarized Raman spectroscopy.

PTh 34

Pulsed EDMR in C$_6$0-films

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In the past years cw-EDMR experiments were successfully performed in thin films of C60 [1], [2]. The EDMR-technique is very sensitive tool to detect spin-dependent processes, therefore it could possibly serve to address and manipulate a few number of spins in an N@C60-based quantum computer. The C60-films were evaporated on a glass substrate with aluminum contacts in UHV and encapsulated in nitrogen atmosphere to protect them against oxygen. Under illumination with an Ar-laser (514 nm, 150 mW), spin-dependent recombination of photo-induced charge-carriers were measured after a pulse-length of 320ns. The spectra showed a resonance at a g-value of g = 2,0020, which is close to the expected one of g = 2,0017 [2]. Using different pulse-lengths from 0 - 1024 ns, we could observe coherent spin-motion (Rabi-oscillations) of a spin-ensemble containing approx. 50000 spin-pairs. At three different microwave intensities the Rabi-oscillations were observed. The width of the Lorentzian shaped FFT of the Rabi-oscillation could be directly related to their damping coefficients. The signal to noise ratio of approx. 10 leads to the assumption that we can reduce the number of oscillating spins by optimizing the sample design by more than one order of magnitude.

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PTh 35

STRUCTURAL TRANSFORMATION OF THE ANTHRACENE TETRAMER TO PICOTUBES

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We present a study of the possibilities to transform the anthracene tetramer into picotubes. Ab-initio DFT studies predicted the possibility to transform the tetramer into a short piece of $(4,4)$ tube by energetic reasons. One possibility for such a transformation is to use a nanotube as template. To explore this possibility, precursor molecules (anthracene) and the anthracene tetramer were studied in conjunction with nanotube systems. Experimentally, Raman spectroscopy with different excitation wavelengths and TEM were used to verify the results obtained.

A high temperature treatment of an anthracene-nanotubes mixture revealed a shift in the Raman lines of the anthracene. This shift is an indication of a successful filling the nanotubes with the molecule.

In the case of the anthracene tetramer, a similar high temperature treatment was used, and the obtained spectra revealed a similar line shift. Selective experimentation and a good agreement between Raman spectra calculated for the short $(4,4)$ tubes are consistent with a transformation process of the tetramer to $(4,4)$ picotubes on the surface of the bundles, but not inside the tubes.

BIOCOMPATIBILITY OF MULTI WALLED CARBON NANOTUBES

PTh 36

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We have investigated the biocompatibility of multi walled carbon nanotubes. The carbon nanotube samples were prepared using various surfactants. By applying nuclear magnetic resonance, the relaxation properties of materials comparable to various kinds of human tissue were studied dependent on the carbon nanotube concentration.

EPR INVESTIGATIONS ON HYDROGEN ATOMS ENCAGED IN SILSESQUIOXANE MOLECULES

PTh 37

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Atoms trapped in molecular cages have recently been proposed [1] as qubit representations for quantum computing. Hydrogen atoms entrapped in cubic silsesquioxanes provide a conceptually simple two-spin system (S=1/2, I=1/2) with a large hyperfine coupling between the 1s electron and the proton. Electron spin relaxation times at room temperature were earlier found to be encouragingly long (T2 8 μs) [2].
We report on synthesis by both radiation chemistry and ion implantation of hydrogen in different Si8O12R8 cages (R = (CH2)nH with n=0-3). Spin properties and relaxation times were investigated using both cw and pulsed EPR measurements. Spin echo modulation (ESEEM) was observed, yielding information about isotropic and anisotropic interactions of the unpaired electron with 29Si nuclei and distant protons.

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Aerosol smog chamber studies of the atmospheric transformation of aerosol-borne ODVE and sea salt

PTh 38

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It is well known that sea salt and particle-borne chemicals are transported over long range by the wind and that the particles and chemicals can be transformed by atmospheric photochemistry during this trasport. To investigate this natural phenomenon, an aerosol smog chamber facility has been set up in a coolable laboratory at temperatures down to -28 °C.
The aerosol particles used in this study were Al2O3 (150 g/m2, Alumina C, Degussa) and sea salt with a typical composition, i.e. NaCl with traces of NaBr.
The aerosol smog chamber used for the study with Al2O3 was made of Duran glass (a vertical cylinder, 3250l) and it was irradiated from the bottom by a solar simulator, consisting of 16 Osram Eversun Super fluorescent lamps, 80W each.
The Al2O3 was coated at sub-monolayer thickness with octadecyl vinyl ether (ODVE, C20H40O, M=296g/mol) and exposed to simulated sunlight at known levels of OH radicals. After that the aerosol was sampled on teflon filters. The filter samples were analyzed by gas Chromatography (GC) for the ODVE content. To identify the products, GC-MS and FTIR spectroscopy were used.
Furthermore, the release of reactive halogenated species from sea salt under arctic (down to -28 øC) and tropospheric conditions was investigated in Teflon (FEP 200A, Dupont) smog-chamber experiments under irradiation by a similar solar simulator.
From the consumption of ozone and hydrocarbons, we are able to evaluate the importance of the participating radicals Br, Cl and OH. Particle size distributions (with a maximum of the number density at 300 nm) were determined, and the average residence time of the salt particles in the suspended state (20h at relative humidities around 30 %) was calculated.

PTh 39

NATURAL CHARGING OF CNTS IN GAS PHASE AND ANALYSIS OF POSSIBLE MECHANISMS

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Spontaneous electrical charging phenomenon of bundles for single-walled carbon nanotubes (CNTs) synthesized with an aerosol (floating catalyst) method was discovered. CNT bundles were both positively and negatively naturally charged whereas individual nanotubes remained electrically neutral. On the basis of the observed self-charging of the nanotubes, a novel method for the separation of individual CNTs from bundles and their subsequent deposition on a wide variety of substrates at ambient temperature was developed.

Analysis of the mchechnims of CNT charging revealed that the charging effect can be explained by the van der Waals energy released during the CNT bundling. A forming bundle can be charged due to the emission of electrons and ions via dissipation of the released energy.

PTh 40

CHARGE DISTRIBUTION OF MOLECULAR FILLED CARBON NANOSTRUCTURES INVESTIGATED BY HIGH-ENERGY SPECTROSCOPY

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Carbon nanostructures such as fullerenes and single wall carbon nanotubes are of great interest because their low-dimensional nanospaces to be filled with various atoms and molecules give us an opportunity to testify issues of the fundamental physics in low dimension as well as to realize fascinating nanodevices. We report on a detailed study of the charge distribution of the fullerenes and SWCNTs with different filling materials, such as endohedral fullerenes, peapods and double-wall carbon nanotubes, by using photoemission, x-ray absorption and electron energy-loss spectroscopy as element-selective probes. Low-energy electronic properties of those nanomaterials are analysed as a function of in-situ doping with alkali metals. This allows us to get further insight on the charge distribution concomitant with excess charge transfer between the filling and the host, as well as possible doping-induced transitions of the metallic states of the SWCNTs from a Tomonaga Luttinger liquid to a normal Fermi liquid.

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PTh 41

Strain and Pressure Sensing with Carbon Nanotubes

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Carbon nanotubes have been demonstrated to behave piezoresistive, i.e. to change resistance dramatically upon elastic deformation [1, 2]. Recently, several demonstrators were shown that utilized this effect for strain sensing, pressure sensing and as a nano electromechanical transducer [3, 4]. These works relied either on direct growth of only one carbon nanotube within a micro- or nanostructure or contacting nanotubes after random deposition on a substrate.

In our work we establish a more robust method for incorporating carbon nanotubes into microsystems based on ac-dielectrophoresis [5, 6]. In contrast to other publications there are severals carbon nanotubes contacted at once. On the cost of sensitivity of the sensing element the reliability is greatly improved. We demonstrate the functionality of our approach with strain gauge and a microsystem pressure sensor.

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Charge transport in carbon nanotubes through surface acoustic waves

PTh 42

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The need of devices able of quantized charge transport on nanoampere scale with very high precision led to several developments in low-dimensional structures. The majority of cases is based on a GaAs-2DEG where the electrons are confined by the electrical potential of the applied surface acoustic wave (SAW). In several recent publications a new SAW-related effect has beeen predicted and investigated. Thereby the function of the 1D conducting channel is taken over by a semi-metallic single-walled carbon nanotube.
The SAW is induced through the the piezoelectric effect. For this purpose lithographically generated metallic interdigital transducers (IDT) are used.
The coupling of SAW's electrical part to the electrons is given by the electron structure in the nanotubes. The aim of the work is to present an overview of theoretical predictions and existing experimental work. The device suitable for detecting the predicted effect will be presented and the experimental progress will be reported.

Luminescence properties of hexagonal Boron Nitride and Single Walled Boron Nitride Nanotubes

PTh 43

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Hexagonal Boron Nitride (hBN) and Boron Nitride Nanotubes (BNNTs) are promising wide band gap semiconductors with potential use in UV optoelectronics. Indeed, recent experimental and theoretical studies on hBN optical properties have shown significant excitonic effects. Because of the presence of contaminants in the samples, optical measurements on BNNTs are much less reported, but BNNTs are also expected to be highly luminescent materials because of excitonic effects.
BN-SWNTs are synthesized by laser vaporization of hBN target in nitrogen atmosphere. The raw material is composed of BN-SWNTs, small hBN particles extracted from the target, solid boron droplets encapsulated into hBN shells and boric acid. This raw material is purified to separate the nanotubes from the other contaminants, and the resulting products are characterized by HRTEM. In contrast to carbon nanotubes, as electronic properties and especially BNNTs band gap do not differ with diameter and chirality, macroscopic measurements of BNNTs optical properties are allowed to determine their luminescent characteristics.
We investigate hBN and BN-SWNTs optical properties by means of variable temperature photoluminescence and cathodoluminescence experiments. The results are in good agreement with theoretical predictions and experimental results concerning the role of excitons on the optical properties of these materials.

Effect of ion irradiation on transport properties of transparent networks made of SWNT

PTh 44

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Thin networks of SWNT of various thicknesses were air-brushed on Si/SiO2 wafers and glass substrates and then irradiated with Ar+ and N+ ions with energy 30 keV. Effect of the doses of ion-irradiation on the structure of SWNT networks was studied.
Raman spectra show changes of intensities of all typical lines, especially the D-line. Increase of the D-line with the rising dose is more pronounced in the case of N+ ion irradiation.
Optical absorption spectra are also influenced by the ion irradiation. The first peak of the Van Hove singularities decreases and shifts to higher energies for both Ar+ and N+ ions.
We measured temperature dependences of the electrical conductance G(T) and I-V characteristics using the four-probe method. The results of the electrical measurements show a decrease of conductance in several orders of magnitude accompanied with a radical change in shape of G(T) after ion irradiation. The change of the conductance is strongly affected by the dose of the ion irradiation and it is similar for both Ar+ and N+ ions while the thinner SWNT networks are more affected than the thickest ones.

PTh 45

PHYSICAL PROPERTIES OF CARBON NANOSTRUCTURES DERIVED FROM FULLERENE C70 AT HIGH PRESSURE

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It has been well established that application of high pressure to C60 at elevated temperatures results in formation of one-dimensional (1D) and two-dimensional (2D) polymeric structures comprised of covalently bonded buckyballs [1]. Nevertheless, numerous attempts to polymerize the next simplest fullerene, C70, have generally been inconclusive and yielded only dimers (C140) [2,3] until the polymer was finally synthesized at hydrostatic pressure in the form of zig-zag chains [4]. Here we present the results of a wide range of experimental studies (Raman, FTIR and NMR spectroscopy, thermal conductivity, high resolution dilatometry) of C140 and 1D polymeric C70. We show that the type of nanostructure (dimers vs. chains) formed during polymerization of C70 at high pressure strongly depends on the structural state of the source material. In a separate set of experiments dedicated to study of the kinetics of de-polymerization of C140 and 1D polymeric C70, we revealed a tremendous difference in the relaxation times for the process in these systems which we tentatively associate with the difference in entropy change during de-polymerization. Polymeric forms of fullerenes have implications for molecular electronic devices. We have measured electron tunneling in single-electron transistors made from C140 and observed its strong coupling to the stretching (inter-cage) vibrational mode [5]. The results are discussed in terms of Frank-Condon model.

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PTh 46

SINGLE-WALLED CARBON NANOTUBE BASED PRESSURE SENSORS

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We report on the design, fabrication and characterization of bulk micromachined pressure sensors based on circular alumina membranes and individual single-walled carbon nanotubes (SWNTs) as the active electromechanical transducer elements. The nano electromechanical sensor consists of an individual electrically-connected SWNT adsorbed on top of a bulk micromachined 100 nm thick atomic layer deposited (ALD) circular alumina (Al2O3) membrane with a radius in the range of $50 - 100\mu m$. We present mechanical, electrical and combined electro-mechanical measurements of the sensor. A white light interferometer (WLI) was used to measure the deflection of the membrane due to a differential pressure. The mechanical properties of the device (including the pure alumina membrane) were characterized by bulge testing methods. We were the first to perform electromechanical measurements on strained metallic SWNTs adhering to a membrane, and found a piezoresistive gauge factor of approximately 210 for metallic single-walled carbon nanotubes, which exceeds the gauge factors of state-of-the-art silicon-based strain gauges.

IMMOBILIZATION OF CNT/CNFS ONTO SURFACE AND INSIDE OF THE MODIFIED ACTIVATED CARBON

PTh 47

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The applications of carbon CNTS/CNFs in chemistry and catalysis require the availability of large amounts of material with well-defined surface chemical and mechanical properties. Loose CNTs/CNFs are unsuitable as they cannot be controlled in their suprastructural properties and operations of compaction can destroy or at least inhibit the access of the reactant medium to the nanostructures. It is mandatory for chemical applications to use only one chemical element for all dimensions of structuring and to avoid the combination of nanocarbon with non-carbon support structures. An ideal substrate is activated carbon from natural sources. Such bio-inorganic polymers are well structured in several dimensions, reactive for modifications and available in masses. The present paper describes ways to modify the activated carbon obtained from the bio-waste of palm oil production as host for the growth of nanocarbon. CNts/CNFs can be immobilized on the outer surface and nested inside of the activated carbon leading to hierarchically structured carbon materials that are highly suitable for sorption and catalytic applications and for binder-filler applications(1).
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SURFACE DEFORMATIONS INDUCED IN SiO2 DUE TO ELECTRON EMISSION DURING ELECTRIC FIELD DIRECTED CVD GROWTH OF CARBON NANOTUBES

PTh 48

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Surface modifications of SiO2 subtrates have been obtained during CVD growth of single walled carbon nanotubes. The CVD process includes applying an electric field to direct the growing nanotubes across gaps between Mo electrodes. The modifications, which have typical dimensions of a few nm in depth and a few hundred nm in width are only observed when the nanotube grows from the negatively biased electrode. We observe three kinds of structures: trenches with side walls containing a nanotube in the centre of the trench, trenches without side walls and bumps with a nanotube lying along the top. We attribute these observations to the Marangoni effect where strong convection currents are induced in the molten SiO2 layer, locally heated by the growing nanotube. Temperatures on the order of 2000 K can be reached in the nanotube when growing from the negatively biased electrode due to strong ohmic heating induced by field emission.

Assembly of Carbon Nanotube Field-Effect Transistors by ac-Dielectrophoresis

PTh 49

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Field-effect transistors (FETs) based on semiconducting carbon nanotubes (CNT) are promising candidates for applications as gas or biosensors or switching devices in a forthcoming molecular electronics. Nevertheless, the reliable strategies for the build-up of these devices are not developed yet.
Recently, a novel method has been introduced which allows the assembly of CNT-bridges between adjacent metal electrodes by ac-dielectrophoresis [1]. Here we use this method for the parallel fabrication of wires of DNA-dispersed CNT [2,3]. To select only the semiconducting paths, we break the metallic tubes electrically [4,5] after the deposition, leading to a reliable and reproducible fabrication of CNT-based FETs.
In our contribution we discuss the electrical performance of the CNT-FETs on air and in liquid solution. Improvement of the devices by their high-temperature treatment is also demonstrated.

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PTh 50

Study of dissociation of tripropylamine and formation of ultra-small single-walled carbon nanotubes inside catalytic channels of Co-AFI zeolite single crystals

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We report our recent study on processes of dissociation of TPA molecules and formation of the ultra-small single-walled carbon nanotubes in the channels of Co-incorporated AFI (Co-AFI) zeolite crystals, by means of mass spectroscopy, Fourier transform Infrared (FTIR) spectra and Raman scattering techniques. In comparison with pure AlPO4-5 crystals, the carbonization temperature of TPA molecules inside the channels of Co-AFI crystals is notably decreased, indicating that Co atoms incorporated in the AFI framework plays an important catalyst role. These incorporated Co atoms are also favorable to the formation of nanotubes in the channels, characterized by a significant decrease in nanotubes formation energy. FTIR spectra in situ measured at temperature 30 - 800 øC showed that TPA molecules decomposed into lighter amines via abstraction of propylene and the stepwise formation of dipropylamine, n-propylamine and ammonia at temperature region 350 - 400 °C, and carbonized at temp eratures above 400 øC. The 0.4 nm nanotubes were formed at about 500 øC. The differential scanning calorimetry (DSC) and Thermogravimetry (TG) results showed that the formation of the ultra-small SWNTs will not come into being, until enough dimers and trimers of carbon form when the C-H bond of propylene (C6H6) or its smaller oligomers break gradually.

PTh 51

BIOMINERALIZATION ON THIN FILMS OF CHEMICALLY FUNCTIONALIZED CARBON NANOTUBES

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Construction of organic-inorganic hybrid materials with controlled mineralization analogous to those produced by nature is now of current interest for both organic and inorganic chemists to seek industrial and technological applications. In bone, calcium phosphate in the form of hydroxyapatite (HA) crystallites deposits within gap regions of the collagen soft matrix. The bone protein has a typical fibrous structure, which acts as a structural framework of the composite material, whereas HA gives the desired rigidity and strength. Over the past four decades, several biomaterials have been developed and used as bone grafts. The fabrication of fibrous scaffolds that mimic the structure and properties of natural bone is a significant challenge since it involves different chemical species that have a specific spatial relation.

This report provides a survey on crystal nucleation and growth of calcium phosphate and calcium carbonate by chemically functionalized carbon nanotubes (CNT) as templates. Due to their structure-dependent unique properties, CNT are extremely promising for applications in materials science. Model systems in which low molecular weight and linear polymeric species are attached onto the CNT graphitic surface are used to study the effect of functionality on inorganic crystallization. To study the template-directed crystal nucleation and growth, thin films of CNT are used as scaffolds. The composition and structure of the minerals is characterized spectroscopically by IR, Raman, XRD and SEM. These interesting results may lead to fundamental developments in areas relating to the biomineralization process, which is expected to be the impetus for the next industrial revolution.

RAMAN INTENSITIES OF THE FIRST OPTICAL TRANSITIONS IN CARBON NANOTUBES

PTh 52

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We performed resonant Raman spectroscopy on the frst optical transitions E11 of separated single-walled carbon nanotubes. In contrast to photoluminescence spectroscopy resonant Raman scattering is independent of the exciton relaxation between different bands. Recent theoretical work shows that the luminescence of nanotubes belonging to the nu=(n-m)mod3=+1 family is weakened by an extra relaxation channel [1]. We collected radial breathing mode (RBM) spectra varying the excitation energy in the infrared between 1.12 and 1.49 eV. An experimental Kataura plot was obtained from resonance profiles and the Raman frequency of each RBM [2]. We discuss the dependence of Raman intensity on the nanotube family nu and the chiral angle. We compare our results to photoluminescence experiments considering the extra relaxation channel [1] and to predictions on the electron-phonon coupling strength [3].

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Solution vs melting filling of single-walled carbon nanotubes

PTh 53

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Single-walled carbon nanotubes (SWNTs) have been advocated as perfect candidates for the sustainable miniaturisation of electronic and mechanical nanoscale devices. More recently there is discussion on their use in medical applications such as drug delivery. Encapsulation within and release of selected compounds from the inner hollow cavity of SWNTs is therefore a key step. Solution and melting filling are two of the most frequently used methods to prepare filled SWNTs (composites). It has been previously reported that many filled SWNTs samples retain their filling material despite vigorous attempts to remove it. For example, samples of alkali halides such as KI inside SWNTs can not be removed after continuous extraction in a Soxhlet apparatus for three weeks. Similar behaviour has also been observed for SWNTs filled with lanthanide halides. Here we present a comparison between solution and melting filling during different steps: filling, removal of the excess of filling material and release of the encapsulated compounds.

Separating spin and charge transport in single wall carbon nanotubes

PTh 54

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We demonstrate spin injection and detection in single wall carbon nanotubes using a 4-terminal, non-local geometry. This measurement geometry completely separates the charge and spin circuits. Hence all spurious magnetoresistance effects are eliminated and the measured signal is due to spin accumulation only. Combining our results with a theoretical model, we deduce a spin polarization at the contacts of approximately 25 %. We show that the magnetoresistance changes measured in the conventional two-terminal geometry are only partly due to spin accumulation.

PTh 55

TRANSPORT PROPERTIES STUDIES OF MOLECULAR DEVICES USING MoSIx NANOWIRES

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Different molecular devices based on MoSIx nanowire systems were measured with the aim to investigate their electronic properties. A variety of techniques for the integration of the MoSix bundles into devices were tested including AC and DC trapping over narrow electrode channels and the manufacture of circuits with bundles half imbedded under a layer of metal. Conductivity of such bare bundle devices is compared to circuits, with golden particles attached to the ends of the bundles, where electrons are injected longitudinally into the wire. A clearer image of the scattering along the tube can be obtained in this case, since in the case of metal-coated bundles, the electron injection mechanism involves transverse coupling. Moreover the contact conductivity in functionalized bundles is easier to extract and therefore better controlled. We report a series of measurements on devices annealed at different temperatures in vacuum and in inert argon atmosphere. The contact conductivity was also tested for different contact metals. We compared devices made using pure gold, nickel, titanium and gold with an underlying layer either of titanium or nickel.

PTh 56

IMPURITY INDUCED INTERTUBE CONDUCTANCE IN DOUBLE-WALL CARBON NANOTUBES

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In double-wall carbon nanotubes a lattice of outer tube is incommensurate with that of inner tube. It has been reported that in such incommensurate double-wall tubes intertube conductance is negligibly small. This is essentially due to difference in momentum between outer and inner tubes. Recently, we clarified that since intertube coupling quasiperiodically oscillates as a function of position, almost all couplings cancel out except those near tube edges, and this incomplete cancellation leads to small intertube conductance, which is typically 10^{-4} in units of the conductance quantum for tubes with 1.5nm in outer tube's diameter. This mechanism well explains that conductance average and fluctuation are independent of the length.

In this paper we numerically study intertube conductance in double-wall tubes with impurities. Calculated results show that intertube conductance is linearly increased with increase of the length, which can reach at ten percent of the conductance quantum, as long as the length is shorter than the localization length. This is because the quasipeirodic oscillation of intertube coupling, that is, cancellation of intertube coupling is disturbed by random impurity potential. The linear length dependence indicates that the conductance is determined by the fluctuation of impurity potential.

PTh 57

STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF Mo-S-I NANOWIRES: A THEORIST'S VIEW

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Quasi one-dimensional materials like nanowires or nanotubes are attracting considerable interest in particular because of their potential applicability in nanoelectronic and nanomechanical devices. Common to all of them is strong uniaxiality in electronic as well as mechanical properties, which is related to weak van der Waals coupling between individual molecular chains.

In this contribution we report on the ab-initio total-energy and band structure calculations and discuss the structural, mechanical, electronic and optical properties of these compounds. The calculations are based on the DFT as implemented in the WIEN2k package and the dielectric and optical properties are calculated in the random-phase approximation. The electron bands have very small dispersion in the plane perpendicular to the wires, the electrons are localized on individual wires and their hopping rates between the neighbouring wires are small. The anisotropy is reflected also in the mechanical and optical properties.

The emphasis will be on the $Mo_6S_3I_6$ compounds which have been synthetised recently and on Mo_6S_6 which, according to our predictions, has extraordinary mechanical and electronic properties.

Spin Active Fullerene Superlattices **PTh 58**

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Endohedral fullerenes possess unique physical and chemical properties which may be useful in next generation nano-electronic devices. We have synthesised ordered endohedral fullerene-based structures in which the unique properties of the incarcerated species are retained. We describe the principles developed for the construction of low dimensional fullerene-based structures and their physical properties as characterised by transmission electron microscopy (TEM) and optical and electron spin resonance (ESR) spectroscopies.

High Modulation Silicon Nanowire Field Effect Transistors **PTh 59**

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Silicon nanowires (Si-NWs) with diameters below 20nm were grown by catalytic chemical vapor deposition. Planar field effect transistors (FETs) were fabricated by implementing the undoped Si-NWs as the active region. The channel is controlled by a common back gate, consisting of a doped substrate covered by silicon-dioxide as the gate-dielectric. Various silicides were investigated as Schottky-barrier source and drain contacts for the active region. For CoSi, NiSi and PdSi contacts, the transistors transfer characteristics of nominally undoped Si-NWs all show p-type behavior. A FET consisting of a single Si-NW with 20 nanometers diameter and 2.5 micrometers length (gate-length) delivers as much as 0.1 microampere on-current at 1 volt bias voltage and has an on/off current ratio of 7 orders of magnitude. The on-current is independent of the gate-length if shorter than 1æm and seems to be limited by the Schottky barriers at the contacts. This is in contrast to recent reports of low conductance in undoped Si. Due to these promising electric properties and the ability to use bottom up processing, a first step in fabricating a vertical Si-NW FET at a predefined position is presented here: For the first time single Si-NWs were grown out of lithographically defined holes.

CARBON NANOTUBE TRANSISTORS ON SELF-ASSEMBLED ORGANIC GATE DIELECTRIC **PTh 60**

Ralf Thomas Weitz, Ute Zschieschang, Hagen Klauk, Marko Burghard, and Klaus Kern
Max-Planck-Institute for Solid State Research, Stuttgart Germany

A silane-based organic self-assembled monolayer was utilized as a gate dielectric on top of a highly doped silicon wafer for individual single-walled carbon nanotube transistors in a back-gate configuration. The use of these monolayers enables device fabrication at low process temperatures (below 200øC) and hence in principle the usage of flexible substrates. In addition this gate dielectric is extremely thin (5nm) which allows a strong gate coupling. The source and drain contacts were fabricated by conventional e-beam lithography, which is performed after the organic monolayer and the carbon nanotubes had been deposited. The gate leakage current I_{gate} of finished devices exposed to an electron-beam dose of 600 æC/cmý did not exceed 106 A/cmý at a gate voltage of 4 V. Transistors exposed to a three times higher e-beam dose during fabrication however, showed an I_{gate} of more than 103 A/cmý. This indicates a damage of the monolayer gate dielectric by the higher e-beam dose. Metallic nanotubes in low-leakage devices measured at 2K show Coulomb oscillations with a period five times smaller than in devices comprising a 200nm SiO_2 gate dielectric.

PTh 61

Local ferroelectric properties of single crystals (CH3NH3)5Bi2Br11 (MAPBB)

M. Wojtas
University of Wroclaw, Poland

Local ferroelectric properties of single crystals (CH3NH3)5Bi2Br11 (MAPBB) are investigated by Scanning Probe Microscopy (SPM) in a piezoelectric contact mode. The SPM signal proportional to the effective piezoelectric coefficient, deff, is measured along with the standard topography. Both ferroelectric domain imaging and local hysteresis measurements are performed at room temperature in the close vicinity of the phase transition temperature (Tc = 39 C). Lamellar domain structure with the phase contrast due to 180 domains is observed for the surfaces perpendicular to the polar direction. Local hysteresis loops acquired by SPM are well saturated with the average coercive voltage of 15 V. The shape of the loops is found to depend on the stiffness of the SPM cantilever. The mechanisms of the domain contrast and prospects of using MAPBB for high-density data storage are discussed.

PTh 62

EFFECT OF AR ION IRRADIATION ON THE FET BEHAVIOR OF SINGLE WALLED CARBON NANOTUBE

Y. Woo[1], Z. Osváth[2], L.P. Biró[2], and S. Roth[1]
[1] Max-Planck Institute for Solid State Research, Heisenbergstra. 1, 70569 Stuttgart, Germany; [2] Research Institute for Technical Physica and Materials Science, H-1525 Budapest, P.O.Box 49, Hungary

Various atomic-scale defects of carbon nanotube (CNT) such as vacancies and pentagon/heptagon Stone-Wales defects have been studied, especially focusing on their effects on the electronic structure of CNT using scanning tunneling microscopy. Recently, Gómez et al. have reported the electronic transport properties of single walled carbon nantoube (SWNT) with creating defects using Ar+ ion irradiation. In this study, we investigated how the characteristics of carbon nanotube field effect transistor changes gradually with Ar+ ion irradiation. Because SWNT is placed on the metal electrode in this experiment, vacancies created by Ar+ ion could exist on the contacting area with the metal electrode as well as the bulk of SWNT. As a result, the conductance obtained from the Isd-Vsd curve was observed to decrease after Ar+ ion irradiation due to the electron scattering at defects. However, for a small bundle of SWNT, the conductance at small Vsd is rather larger at 4K and the gate dependence exhibits more metal-like behavior after Ar+ ion irradiation. In next, only the contacting area between SWNT and metal electrode was exposed to Ar+ ion irradiation, and then the Isd-Vsd measurement was performed in order to see the role of defects on the contact properties between SWNT and metal electrode.

PTh 63

FUNCTIONALIZATION OF SINGLE-WALLED CARBON NANOTUBES BY A NEW ALKYLATION-OXIDATION PROCESS

David Wunderlich[1], Jürgen Abraham[1], Ralf Graupner[2], Lothar Ley[2], and Andreas Hirsch[1]
[1] Institute of Organic Chemistry, Henkestraáe 42, Erlangen, Germany; [1] Institute of Technical Physics, Erwin-Rommel-Straáe 1, Erlangen, Germany

We have found a new method for a preferred alkylation of metallic single-walled carbon nanotubes (m-SWCNTs) to semiconducting single-walled carbon nanotubes (s-SWCNTs). The first reaction-step is the covalent attachment of alkyl moieties by an alkyl-lithium compound, such as tert-butyl-lithium, producing a well dissolved lithium-nanotube salt. The second step is the oxidation of this species by bubbling oxygen through the homogenous solution under precipitation of the functionalized nanotubes. The repetition of these steps without further purification overcomes the limited first alkylation step and yields highly sidewall-functionalized nanotubes that are soluble in common organic solvents. The effective debundling of the nanotubes was revealed by atomic force microscopy (AFM) and transmission electron microscopy (TEM). The elemental composition of the functionalized SWCNTs was determined by X-ray photoelectron spectroscopy (XPS). Raman spectroscopy revealed the preferred alkylation of the m-SWCNTs by a decrease of the intensity of the radial breathing modes (RBM) in the metallic region.

TAILORED SYNTHESIS OF DOUBLE WALLED CARBON NANOTUBES BY SUPER-GROWTH

PTh 64

Takeo Yamada[1], Tatsunori Namai[1], Kenji Hata[1], Don N. Furaba[1], Kohei Mizuno[1], Jing Fan[2], Masako Yudasaka[2,3], Motoo Yumura[1], and Sumio Iijima[1]
[1] Research Center for Advanced Carbon Materials, National Institute of Advanced Industrial Science and Technology (AIST); [2] Japan Science and Technology Agency, 3 NEC Corporation

We have succeeded in synthesizing vertically-aligned double-walled carbon nanotubes (DWNT) forests with a height up to 2.2mm by water-assisted chemical vapor deposition (we called it Super-Growth CVD). In this presentation, we will show how one can tailor the catalysts to achieve high and maximized selective growth of DWNTs by Super-Growth CVD. First, a phase diagram of the relative population of SWNT, DWNT, and MWNT vs. the tube diameter grown from Fe thin films as a catalyst was constructed from hundreds of TEM images. Second, we found that the average tube diameter is roughly proportional to the thickness of the Fe thin film catalyst. Combined with the phase diagram, we arrive at a direct way to engineer the relative proportion of SWNTs, DWNTs, and MWNTs by tailoring the catalyst thickness. More importantly, we can find exactly the optimum catalyst thickness to maximize the proportion of DWNTs. Our best result is 85% DWNTs in the as-grown material, representing one of the highest, if not the highest, reported selectivity towards DWNT synthesis.

Field Electron Emission Properties of Multiwall Carbon Nanotube Yarns

PTh 65

A.A. Zakhidov[1], M. Zhang[2], A.N. Obraztsov[1], A.A. Zakhidov[2], and R.H. Baughman[2]
[1] Physics Department, Moscow State University, Moscow, Russia; [2] Nanotech Institute, University of Texas at Dallas, Texas, USA.

We report the results of the study of field emission (FE) properties of novel material: multiwall carbon nanotube (MWCNT) spun yarns. The MWCNT yarns produced by method developed in UTD have unique mechanical properties [1]. FE characteristics were obtained for lateral surface of MWCNT yarns and for their ends. Very low FE threshold of about 0.9 V/um and uniform distribution of emission sites were found for surface of the yarns. Such lateral electron emission is suitable for application in flat panel displays and lighting elements. Very high emission current density (up to 1000 A/cm2) has been achieved for single end emitters made of MWCNT yarn. The electron emission was accompanied by incandescence of the yarn ends and intensive light emission with spectral characteristics corresponding to heating temperature of about 2200K.

[1] M. Zhang, K. R. Atkinson, R. H. Baughman: Science 306, 1358 (2004).

TRANSPARENT CARBON NANOTUBE SHEETS FOR OLED AND SOLAR CELLS

PTh 66

A.A. Zakhidov, S. Lee, C.D. Williams, M. Zhang, S. Fang, and R.H. Baughman
University of Texas at Dallas

We report the results of the study of field emission (FE) properties of novel material: multiwall carbon nanotube (MWCNT) spun yarns. The MWCNT yarns produced by method developed in UTD have unique mechanical properties [1]. FE characteristics were obtained for lateral surface of MWCNT yarns and for their ends. Very low FE threshold of about 0.9 V/um and uniform distribution of emission sites were found for surface of the yarns. Such lateral electron emission is suitable for application in flat panel displays and lighting elements. Very high emission current density (up to 1000 A/cm2) has been achieved for single end emitters made of MWCNT yarn. The electron emission was accompanied by incandescence of the yarn ends and intensive light emission with spectral characteristics corresponding to heating temperature of about 2200K.

[1] M. Zhang, K. R. Atkinson, R. H. Baughman: Science 306, 1358 (2004).

PTh 67

CARBON NANOTUBE FIELD EFFECT TRANSISTOR OPERATION AT 23GHZ

Hong Zhang, Aaron Pesetski, James Baumgardner, Jim Murduck, John Przybysz, and John D. Adam
Northrop Grumman Corporation, Linthicum, US

Carbon nanotube field effect transistors (CNT FETs) are being developed as potential replacements for silicon and III-V semiconductor devices for high frequency electronics applications. CNT FETs have demonstrated the highest carrier mobility at room temperature of any known material and high electrical and thermal conductivity, along with their small size and low parasitic resistances, making them ideally candidates for miniaturized, low-power devices that are capable of operation up to THz frequencies. The development of CNT FETs that operate at high frequencies enables a wide variety of new applications, from high-speed digital logic to spectroscopy of biological molecules.

In this presentation, we will report on our development of CNT FETs, including the device design, growth, fabrication and characterization. A top-gated carbon nanotube (CNT) field-effect transistor (FET) was fabricated on a quartz substrate using a single nanotube grown by CVD and a sputtered SixNy gate dielectric. The frequency-independent performance of a CNT FET, at frequencies as high as 23 GHz, was demonstrated for the first time. This observed operating frequency represents a significant breakthrough in the realization of carbon nanotube-based electronics for high frequency applications.

PTh 68

THEORETICAL INVESTIGATION OF CHARGE TRANSFER BETWEEN THE LAYERS OF DOUBLE WALLED CARBON NANOTUBES

V. Zólyomi[1,2], A. Rusznyak[3], J. Kürti[3], A. Gali[4], A. Szabados[2], and P.R. Surjan[2]
[1] MTA-SZFKI, P. O. B. 49, H-1525, Budapest, Hungary; [2] Dept. of Theo. Chem., ELTE, Pazmany P. setany 1/A, H-1117 Budapest, Hungary; [3] Dept. of Biol. Phys., ELTE, Pazmany P. setany 1/A, H-1117 Budapest, Hungary; [4] Dept. of Atomic Phys., BME, Budafoki ut 8, H-1111, Budapest, Hungary

The physical properties of several kinds of double walled carbon nanotubes are investigated with density functional theory and the intermolecular Huckel model. We find that electrons are transferred from the outer wall to the inner wall in all cases, with the magnitude of the charge transfer slightly varying with the chirality of the inner tube. For metallic band structures, a large density of states is found at the Fermi level as a consequence of the charge transfer. The possibility of nearly universal metallicity of double walled nanotubes is discussed, in light of recent NMR measurements.

PTh 69

TiO2(B) NANOTUBES PREPARED VIA NOVEL SYNTHETIC ROUTE AND THEIR ELECTROCHEMICAL AND PHOTOCATALYTIC PERFORMANCE

Marketa Zukalová, Martin Kalbác, Ladislav Kavan, Ivan Exnar, Andreas Haeger, and Michael Graetzel
1J. Heyrovskì Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejskova 3, CZ-18223 Prague 8, Czech Republic

Novel TiO2(B) nanotubes synthetic route employing amorphous TiO2 as a precursor was developed. The phase purity, stability and electrochemical performance of the product is superior to the TiO2(B) made by the traditional synthesis from K2Ti4O9. Kinetic analysis of cyclic voltammogram revealed that TiO2(B) accommodates Li via pseudocapacitive faradaic process, basically different from the diffusion-controlled lithium storage in anatase or rutile. The reaction rates of the total oxidation of propane per unit of the BET surface area of both TiO2(B) and standard Hombifine N were comparable. In case of the photocatalytic reduction of NO to N2 the quantum yields for TiO2(B) and Hombifine N are proportional to their BET surface areas, but TiO2(B) nanotubes exhibit higher selectivity in the photocatalytic reduction of NO.

Single molecule experiments and non carbon nanophases

8:30 – 9:00	**H.S.J. van der ZANT, NL** *Three-terminal transport through molecular junctions*
9:00 – 9:30	**A. YACOBY, IL** *Measurement of the conductance of single conjugated molecules*
9:30 – 10:00	**F. von OPPEN, D** *Pair tunneling through single-molecule junctions*
10:00 – 10:30	**Coffee break**
10:30 – 11:30	**A. LOISEAU, F** *C-N and C-BN single wall nanotubes: growth and structural properties*
11:30 – 12:00	**G.S. DÜSBERG, D** *Silicon nanowires as electronic devices: CVD growth and characterisation*
12:00 – 12:30	**V.Y. PRINZ, RU** *Ultra-precise molecularly thin semiconductor shells: from nanotubes to nanocorrugated quantum Systems*
12:30 – 17:00	**Mini Workshops**

Application, biology

17:00 – 17:30	**A. BRUININK, CH** *In vitro evaluation of possible adverse effect of nanosized materials*
17:30 – 18:00	**A.T. JOHNSON, US** *DNA-decorated carbon nanotubes for chemical sensing*
18:00 – 18:30	**E. ARTUKOWICH, US** *Carbon nanotube networks as a material for probing biological interactions*
18:30 – 19:00	**T. PICHLER, D** *Concluding Remarks*

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Three-terminal transport through molecular junctions

8:30 SME 1

H.S.J. van der Zant
Kavli Institute of Nanoscience Delft

With electrochemical etching and electromigration, nanogaps on an aluminum gate electrode have been made and small organic molecules of different lengths have been trapped between the electrode pairs. Temperature-dependent transport measurements as a function of gate voltage show that the molecules are weakly coupled to the leads. Samples with the same molecule share common features. For some molecular systems, we find that at low temperatures smaller molecules are worse conductors than longer ones. Asymmetric junctions with a sulfur-gold bonding only on one side, exhibit current-voltage characteristics with steps that are absent for symmetric ones. Coulomb blockade measurements on OPV-3 and OPV-5 show excited states and Kondo behavior. The excitations are associated with vibrational modes and a very good correspondence with Raman spectra is found. Excitations in the single-molecule magnet Mn-12 (S = 10 ground state) are related to non-degenerate spin states. Negative differential resistance and complete current suppression at low bias are explained by a new kind of spin blockade.

Measurement of the conductance of single conjugated molecules

9:00 SME 2

Amir Yacoby
Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

Electrical conduction through molecules depends critically on the delocalization of the molecular orbitals, and their weight on the metallic contacts. Thiolated conjugated organic molecules are therefore often considered as good candidates for molecular conductors. In such molecules the orbitals are delocalized throughout the molecular backbone, with substantial weight on the sulfur-metal bonds. However, their relatively small size, typically 1 nm, calls for innovative approaches to realize a functioning single molecule device. In this paper we report a new approach for contacting a single molecule and use it to study the effect of localizing groups within a conjugated molecule on the electrical conduction. Our method is based on synthesizing a dimer structure, consisting of two gold colloids connected by a di-thiolated short organic molecule, and electrostatically trapping it between two metal electrodes. We study the electrical conduction through three short organic molecules: A fully conjugated molecule, 4,4'-biphenyldithiol (BPD), 4,4'-biphenyletherdithiol (BPED) in which the conjugation is broken at the center by an oxygen atom, and 1,4-benzenedimethanethiol (BDMT), where the conjugation is broken near the contacts by a methylene group. We find that the oxygen in the BPED and the methylene groups in the BDMT suppress the electrical conduction relative to the BPD.

Pair tunneling through single-molecule junctions

9:30 SME 3

Felix von Oppen
Institut fuer Theoretische Physik, Freie Universitaet Berlin, Arnimallee 14, 14195 Berlin

By a polaronic energy shift, the effective charging energy of molecules can become negative, favoring ground states with even numbers of electrons. Here, we show that charge transport through such molecules near ground-state degeneracies is dominated by tunneling of electron pairs which coexists with (featureless) single-electron cotunneling. Due to the restricted phase space for pair tunneling, the current-voltage characteristics exhibits striking differences from the conventional Coulomb blockade. In asymmetric junctions, pair tunneling can be used for gate-controlled current rectification and switching.

10:30
NCNT 1

C-N and C-BN single wall nanotubes: growth and structural properties

A. Loiseau[1], S. Enouz[1,2], O. Stéphan[3], and J.L. Pfeiffer[4]
[1]LEM, ONERA-CNRS, BP72, 92322 Châtillon Cedex , France

Playing on chemical composition of nanotubes is expected to be a very promising route for tuning electronic and optical properties. Whereas carbon nanotubes (CNTs) are metallic or semi-conducting depending on their helicity, boron nitride nanotubes (BNNTs) are wide band gap semiconductors with potential use in UV optoelectronics. For both kinds of tubes, strong excitonic effects have been demonstrated. Mixing both kinds of tubes or doping CNTS with B and/or N could lead to new kinds of tubes with original properties.

In this framework, the vaporization laser method developed at Onera has been shown to be very efficient for synthesizing C-SWNTs and BN-SWNTs [1]. In this work, it has been used for synthesizing for the first time C-Nx SWNTs with different concentrations, x, in nitrogen and C-BN SWNTs. Structure of these tubes and spatial distribution of C, B and N as well as their chemical environments have been inspected at the nanometer scale by combining high resolution transmission microscopy and nano-electron energy loss spectroscopy. These analyses provide clear evidence of new kinds of arrangements of C, B and N within the graphene layer [2]. The mechanisms of formation and growth of these structures as well as their potential properties will be discussed.

[1] R. S. Lee et al, Phys. Rev.B Rapid Comm. 64, 121405 (2001).
[2] S. Enouz et al submitted to Nanoletters (2005).

11:30
NCNT 2

Silicon nanowires as electronic devices: CVD growth and characterisation

G.S. Düsberg, W.M. Weber, F. Kreupl, L. Geelhaar, and H. Riechert
Infineon Technologies AG, Memory Products

Quasi one dimensional structures such as Carbon Nanotubes (CNTs) and Silicon Nanowires (SiNWs) have great potential as beyond the roadmap electronics and optical devices, as shown in numerous experiments. However, the integration and their processability remains a critical issue, especially because of the lack over control of the electronic behavior of CNTs. In this respect SiNWs are much easier to handle, since they have inherent internal structure. Furthermore, the temperature budget for their growth is much lower, doping and contact engineering seems to be possible. In this context our efforts in the field of SiNW integration is reviewed. We report the CVD growth of SiNWs on various substrates down to very low temperatures. Microscopic analysis reveals the single crystal nature of the SiNWs. The diameter can be varied between 2 – 50 nm, and the direction of growth is influenced by the substrate surface. Optical characterizations indicate quantum confinement effects. Planar field effect transistors (FETs) were fabricated by implementing individual undoped SiNWs as the active region. Various silicides were investigated as Schottky-barrier source and drain contacts for the active region. High on-currents and on/off ratios as big as 7 orders of magnitude were measured.

Ultra-precise molecularly thin semiconductor shells: from nanotubes to nanocorrugated quantum Systems

12:00
NCNT 3

V.Y. Prinz
Institute of Semiconductor Physics, The Siberian Branch of Russian Academy of Sciences

Nowadays the new approaches to high-precision fabrication of nanodevices are in urgent demand. There are two alternative strategies for precise nanoobjects fabrication: one strategy is based on controllable formation of precise objects atom by atom, molecule by molecule, while the other one implies application of already pre-assembled precise building blocks. In our previous works[1-3] we have invented a novel approach based on usage of molecular monolayers of solid-state crystal as initial building blocks for fabrication of various micro- and nanoshells (tubes, corrugations, scrolls, fibers, rings, helices, etc.). We have already shown that ultra-thin epitaxial heterofilms (down to two monolayers for InGaAs/GaAs) can be controllably detached from substrates and rolled or buckled in the form of micro- and nanoshells under the action of internal lattice mismatch strains [1]. The diameter of obtained tubes was up to 2 nm[1], nanocorrugated systems had period up to 10 nm[3].

The present review outlines the cornerstone stages of this fabrication technology for semiconductor and metal nanoshells. Considered approach allows making three-dimensional micro- and nanostructures from semiconductor, metal and dielectric films (InGaAs/GaAs, InSbAs/InAs, InP/InAs, Si/GeSi, Si/GeSi/Si3N4/Cr, InAs, Au/Ti, Ta2O5/GaAs and others). New experimental and theoretical results on quantum confinement[4] and quantum transport in semiconductor and hybrid nanotubes, helices, bucklings, corrugations are presented. It was shown, that this molecular technology has a great potential for making materials with new electrical, mechanical, chemical and quantum properties; three-dimensional highly-ordered systems of interacting nanoobjects.

[1] V.Ya.Prinz et all, Physica E 6 (2000) 828-831
[2] V.Ya.Prinz, Physica E 23 (2004) 260-268
[3] V.Ya.Prinz, Physica E 24 (2004) 54-62
[4] V. M. Osadchii and V. Ya. Prinz, Physical Review B 72, (2005) 033313

17:00 APPLb 1 In vitro evaluation of possible adverse effect of nanosized materials

P. Wick, P. Manser, and A. Bruinink
Lab for Materials – Biology Interactions, EMPA Materials Science and Technology, Lerchenfeldstr. 5, CH-9014 St. Gallen

Nanoscaled materials (particles, fibres)(Np) are increasingly used in a wide range of areas, including chemistry, physics, electronics, materials science and the biomedical sciences. As a result environmental, occupational and public exposure to engineered nanoparticles might increase dramatically in the near future as a result of the widespread use of nanoparticles for consumer and industrial products. So far the extent of future exposure to nanoparticles associated with these new products is unknown (SCENIHR, 2005). The discussion regarding the potential risks of their widespread use are just beginning to emerge. In order to make a correct risk assessment of these materials and to elucidate the toxicomechanism comparative in vivo and in vitro research have to be performed using highly characterized Np materials. In our lab a set of Np were investigated in vitro regarding their adverse effects on a variety of cells. To ensure a defined exposition of all cells methodologies were developed to homogeneously and stable disperse Np. Cell culture DNA content, cell activity, quantity of reactive oxygen species but also gene activity were taken as measures to asses the effects.
In the present talk beside a quick overview on risk assessment a short overview on the current state of the art regarding Np toxicity will be given. Furthermore, first Np toxicity data of our lab will be presented.

17:30 APPLb 2 DNA-decorated carbon nanotubes for chemical sensing

A.T. Johnson, A. Gelperin, C. Staii, and M Chen
Univ of Pennsylvania (ATJ, CS, MC) and Monell Chemical Senses Center (AG)

We demonstrate a new, versatile class of nanoscale chemical sensors based on single-stranded DNA (ssDNA) as the chemical recognition site and single-walled carbon nanotube field effect transistors (swCN FETs) as the electronic read-out component. SwCN FETs with a nanoscale coating of ssDNA respond to gas odors that do not cause a detectable conductivity change in bare devices. Sensor responses differ in sign and magnitude for different gases, and can be tuned by choosing the base sequence of the ssDNA. The new sensors detect a variety of odors, with rapid response and recovery times on the scale of seconds. The sensor surface is self-regenerating: samples maintain a constant response with no need for sensor refreshing through at least 50 gas exposure cycles. This remarkable set of attributes makes sensors based on ss-DNA decorated nanotubes very promising for “electronic nose” and “electronic tongue” applications ranging from homeland security to disease diagnosis. Published as C. Staii et al., Nano Letters 5, 1774 - 1778 (2005).

18:00 APPLb 3 Carbon nanotube networks as a material for probing biological interactions

Erika Artukovic[1], Mikhail Briman[1], Wenzhang Xie[2], Lee Goodglick[2], and George Gruner[1]
[1]UCLA Department of Physics and Astronomy; [2]UCLA Department of Pathology and Laboratory Medicine

Combining biological materials and carbon nanotube networks in a resistor or transistor configuration in an active electronic device opens up opportunities for electronic monitoring and possibly control of biological processes. In order to understand more fully the fundamental interaction of proteins with carbon nanotube networks, non-specific binding studies have been conducted. These studies prove there is a charge transfer between proteins and the nanotube network. Cells and viruses have also been integrated into nanotube network devices in an effort to probe the electronic properties of such interfaces.

Concluding Remarks **18:30 CORE**

Thomas Pichler
Leibniz Institute for Solid State and Materials Research Dresden, IFW Dresden, P.O. Box 27016 D-64979;01171 Dresden, Germany

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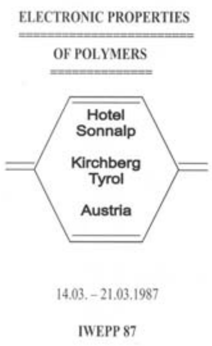
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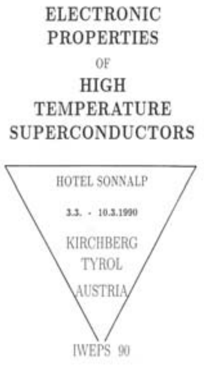
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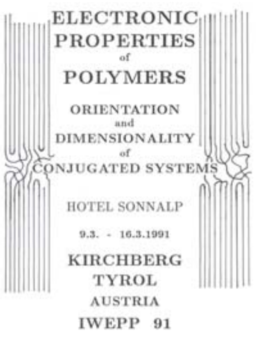
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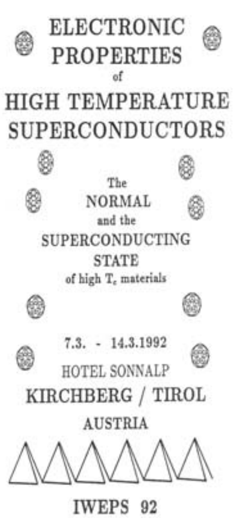
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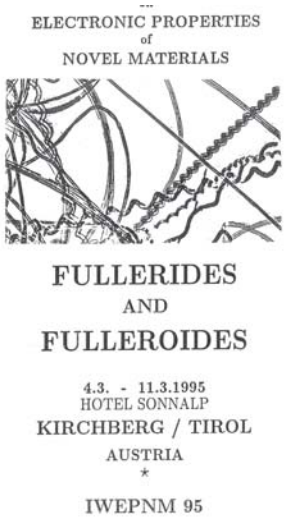
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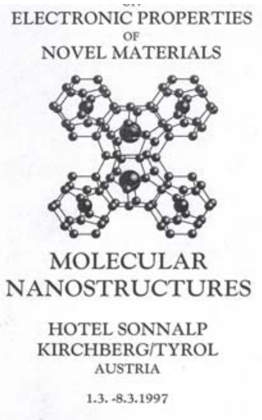
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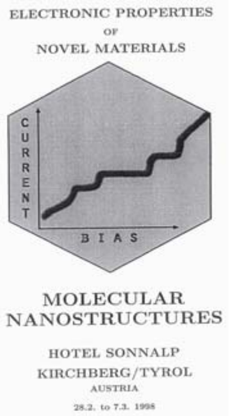
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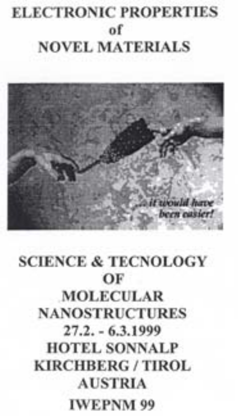
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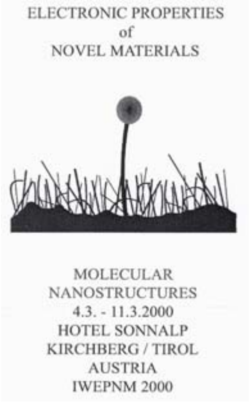
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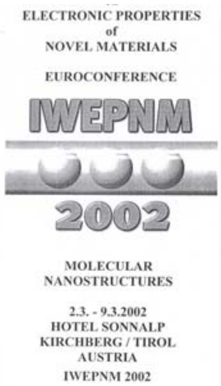
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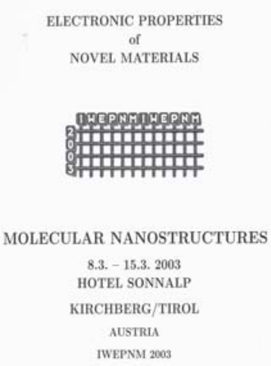
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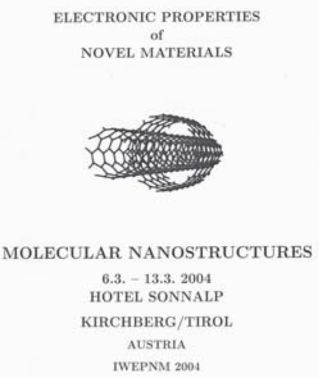
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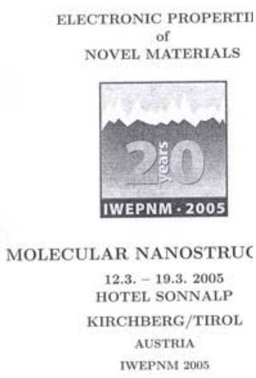
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