SUPPORTERS

Verein zur Förderung der Internationalen Winterschulen in Kirchberg Austria

PATRONAGE

Ewald Haller Bürgermeister von Kirchberg

SPONSORS

Applied Nanofluorescence, 3701 Kirby Drive, Suite 994, Houston, TX 77098, USA Bruker Optik GmbH, Rudolf-Plank Str. 27, 76275 Ettlingen, Germany HORIBA Jobin Yvon GmbH, Neuhofstrasse 9, 64625 Bensheim, Germany Wiley-VCH Verlag GmbH & Co. KGaA,

Boschstraße 12, 69469 Weinheim, Germany

SINEUROP Nanotech GmbH,

Kernerstr. 34, 70182 Stuttgart, Germany

Graphene Industries Limited,

32 Holden Avenue, Whalley Range, Manchester M16 8TA, United Kingdom

The financial assistance from the sponsors and supporters is greatly acknowledged.



Dear Friend:

Welcome to the $22^{\rm nd}$ International Winteschool on: Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of twenty-one 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. It is a tradition of the Winterschools in Kirchberg that this exchange is not restricted to the lectures and poster sessions but occurs throughout the whole week.

The Winterschool is dedicated to molecular nanostructures as a new class of materials. Like the previous Winterschools it runs on an informal level.

If you have any questions concerning the organization and the program, come and see one of us or one of the colleagues involved in the preparation of the meeting. These persons are:

Matthias Müller accomodation Nils Rosenkranz registration

Marcel Mohr video transfer and recording

Hagen Telg general assistance

Harald Scheel receipts, technical assistance

Dirk Heinrich technical assistance Norman Tschirner computer, internet

Also the managers of the hotel, Frau Mayer and her son Herr Mayer, and their staff promised to help us wherever they can. We want, at this point, to acknowledge their help and also that of Janina Maultzsch and María Machón, in the organization of the IWEPNM 2008. We also thank Jannik C. Meyer for his help in designing the logo of this year's Winterschool.

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

Sincerely yours,

Christian, Peter, Hans and Siegmar

Chairmen

- C. Thomsen (Berlin)
- P. Dinse (Darmstadt)
- H. Kuzmany (Vienna)
- S. Roth (Stuttgart)

Program Committee

A. Bachtold (F) P. Dinse (D) M.S. Dresselhaus (US) J.E. Fischer (US) L. Forró (CH)	M. Mehring (D) K. S. Novoselev (UK) M. E. Obraztsova (RU) Th. Pichler (D) J. Robertson (UK)
A. Hirsch (D) S. Iijima (JP) H. Kataura (JP) P. Kouwenhoven (NL)	S. Roth (D) A. Rubio (E) P. Rudolf (NL) C. Schönenberger (CH)
H.W. Kroto (UK) H. Kuzmany (A) Y. H. Lee (KR) A. Loiseau (F) F. Mauri (F)	N. Shinohara (JP) Z.K. Tang (CN) C. Thomsen (D) A. Zettl (US) D. Zhu (CN)

Scope

This winterschool will provide a platform for reviewing and discussing new developments in the field of electronic properties of molecular nanostructures and their applications. Subjects included are: \bullet Carbon nanotube growth and selection \bullet Carbon nanotube spectroscopy \bullet Material science of graphene \bullet Molecular nanostructure transport and spintronics \bullet Theory of molecular nanostructures \bullet Applications of molecular nanostructures \bullet Molecular machines and molecular motors \bullet Template grown molecular nanomaterials \bullet Single-molecule experiments

INFORMATION FOR PARTICIPANTS

Time and location

The IWEPNM 2008 starts on Saturday, March 1, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, March 8, breakfast. There will be a reception party on March 1, after dinner and a farewell party including dinner on Friday, March 7.

Transport

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

Addresses

The address of the Winterschool is:

IWEPNM 2008, Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

Tel: ++43 5357 27410, Fax: ++43 5357 2741 200

e-mail: info@hotelsonnalp.info, Web: www.tiscover.at/sonnalp.parkhotel All questions concerning the the IWEPNM 2008 should be directed to:

Prof. C. Thomsen, Institut für Festkörperphysik, Technische Universität Berlin

Hardenbergstr. 36 10623 Berlin, Germany

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

email: iwepnm-info@physik.tu-berlin.de

Web: http://www.iwepnm.org

Participation

Participation at the IWEPNM 2008 is possible for students and scientists working in the field covered by the scope of the meeting. Because of the limited space the participation requires prearranged acceptance by the organizers.

Contributions

All oral contributions will be presented in the big seminar room of the Hotel Sonnalp. Participants are invited to contribute comments to research and tutorial lectures where 10 minutes for discussion are reserved after each lecture. Beamer presentations, overhead projections and presentations using data video projection will be possible. Presentation of video films needs prearranged confirmation. Invited speakers please test the beamer projection with the technical staff at the latest a few minutes before the session begins. Posters will be presented in the hall of the seminar room.

During the conference

If you want to buy a ticket for the ski lifts in the Kirchberg/Kitzbühel area, please ask at the hotel reception on Saturday evening. Internet connection through WLAN

is available for all participants, even if they are not accommodated at the Hotel Sonnalp. Please check at the front desk.

Proceedings

The contributions to the IWEPNM 2008 will be published by physica status solidi. The expected date for the appearance of the proceedings is September 2008. Contributions can only be published if they arrive before the 30th of April. For the first time an online submission system will be used, which you can find under the following address: http://conferences.wiley-vch.de/v3. The manuscripts will be reviewed within the following weeks. Acceptance of a contribution for presentation at the Winterschool does not automatically include acceptance for publication in the proceedings.

Manuscript preparation

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

- Your manuscript should be written using our Word
 http://www.wiley-vch.de/vch/journals/2231/public/pss_abc_2008_word.zip
 or LaTeX
 http://www.wiley-vch.de/vch/journals/2231/public/pss_abc_2008_latex.zip
 template.
- Relevant PACS numbers (a maximum of six codes) must be given, see the full
 and most recent classification system (PACS 2008) at http://www.aip.org/pacs.
 Always use the complete form, such as 32.50.+i, 71.70.Ej. The page limit for
 invited oral talks is 6 for poster contributions 4 pages. Submission deadline
 is April 30, 2008.

Manuscript submission

For online submission please go to http://conferences.wiley-vch.de/v3. Your login details will be emailed to you by the conference organizers in due time. Select PHYSICA STATUS SOLIDI as the journal and choose IWEPNM 2008 from the list of projects. Once you there, click on "Create manuscript" on the left side of the screen and follow the instructions.

File names

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

IWEPNM 2008 CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 2.03.	morning morning, after coffee break evening	Kuzmany Reich Ferrari
Monday, 3.03.	morning morning, after coffee break evening	Kürti Kataura Forró
Tuesday, 4.03.	morning morning, after coffee break evening	Mauri Maruyama Suenaga
Wednesday, 5.03.	morning morning, after coffee break evening	Robertson Obraztsova Roth
Thursday, 6.03.	morning morning, after coffee break evening	Loiseau Hirsch Hata
Friday, 7.03.	morning morning, after coffee break evening	Briggs Mann Dinse

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 questions from the sideroom (bar)!

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

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

We acknowledge your support.

The Organizers

Final Program

	Sunday 2 March	Monday 3 March	Tuesday 4 March	Wednesday 5 March	Thursday 6 March	Friday 7 March
Topics:	NT optics, Raman	Graphene/ Molecular Electronics	NT transport, Devices	Non-carbon materials, Fullerenes, DWNT	Growth	Quantum Interactions
8:30	Props. of Graphe Graphene Nanor	Novel Electronic and Optical Props. of Graphene and Graphene Nanoribbons LOUIE	Quantum Transport in	Catching Waves and Particles With Nanoscale Resonators ZETTL	Optical Properties of Metallic and Semiconducting SWCNTs KATAURA	Electron Spin Resonance of carbon-based nanostuctures FORRÓ
9:00	Understanding the Nature and Dynamics of Optically Excited States in CNTs HEINZ	Quasiparticle dynamics in Carb	Carbon Nanotubes CHARLIER	Understanding the formation of C-SWNT via in situ and ex situ diagnostics in laser vaporization and CVD techniques LOISEAU		Device Electronics Based on Nanowires and Nanotubes MANN
9:30	Exciton Dynamics, Localization and Transfer in Single Carbon Nanotubes HARTSCHUH	Unravelling the electronic structure of intercalated graphite: a key to graphene and SWCNTs GRÜNEIS	The One-Dimensional Wigner Crystal in Carbon Nanotubes BOCKRATH	-0-3-x x3	Interconnects ROBERTSON	Switchable $ErSc_2N$ rotor within a C_{80} fullerene cage: an EPR and PL study MORTON
10:00			Coffee	break		
10:30	Excitonic imaging spectroscopy of individual single-walled carbon nanotubes LEFEBVRE	Potential barriers in graphene HUARD	Soft Materials with Carbon- Rich Nanostructures FUKUSHIMA	Carbon Nanotubes: Controlled Assembly of	Supply the World with	Graphene single electron transistors ENSSLIN
11:00	Plasmonic nanostructures in aperture-less scanning near field optical microscopy (aSNOM) VOGELGESANG	Observation of Spin-Orbit Coupling in Clean Carbon Nanotubes ILANI	Raman spectroscopy of	Fullerenes and Carbon	in carbon nanostructures SUENAGA	Optical Switching of Porphyrin-Coated Silicon Nanowire Field Effect Transistors WINKELMANN
11:30	Probing the doping in metallic and semiconducting CNTs by Raman MAURI		Plastic Bending Deformation of Carbon Nanotubes NAKAYAMA	Study of Nano-Carbons by Aberration Corrected Low Voltage Electron Microscopy. U. KAISER	The Importance of Defects in CNTs: How to Identify them using Different Techniques TERRONES	Spin Gap and Luttinger Liquid Description of the NMR Relaxation in Cns DORA

12:00 - 17:00	Mini workshops					
17:00 - 18:30	Dinner		17:00 Single Electron Spin Micros-			
18:30	Anharmonic Phonon Lifetimes in Carbon Nanotubes RAO	Graphene spintronics JOZSA	Nanotube ElectroMechanics BACHTHOLD	Catalysis Chemistry of the Confined Nano-Systems BAO	and applications of monodisperse SWNTs	cope: the prospects of adding chemical information to AFM images. HOLCZER
19:00	properties of doped carbon	Ab initio design of reallistic nanotube sensors DA SILVA	SWNT Functional Structures in Sensors HIEROLD	Modification of CNT Architectures for Alternative Energy Applications MINETT	carbon nanotubes	17:30 Detection of single electron spins in N@C ₆₀ molecules HARNEIT
19:30	magnetic resonance studies of CNTs SIMON	Molecular junctions formed by break-junction techniques: electrical conductance determination at a single- molecule scale		Gallium Nitride Nanowires: Impurity and Disorder Effects on Thermal Conductivity FISCHER	detection	18:00 IWEPNM08 - Conference Summary PICHLER 18:30 - 20:00
20:00	Wide-range optical spectra of carbon nanotubes: a	GONZALES Optics of electric flows in graphene. FALKO	Poster Session TUE	Mode-locked 177-fs soliton erbium-doped fiber laser based on a cellulose polymer film containing SWNT synthesized by the arc- discharge method TAUSENEV	Poster Session THU	Break Bauernbuffet Farewell
20:30						
Topics:	NT optics, Raman	Graphene/ Molecular Electronics	NT transport, Devices	Non-carbon materials, Fullerenes, DWNT	Growth	Quantum Interactions
	Sunday 2 March	Monday 3 March	Tuesday 4 March	Wednesday 5 March	Thursday 6 March	Friday 7 March

PROGRAM

AND

ABSTRACTS

solidi Solidi



Solid State at Its Best



2008. Volume 205, 12 issues. Print ISSN 0031-8965 • Online ISSN 1521-396X 2008. Volume 245, 12 issues.
Print ISSN 0370-1972 • Online ISSN 1521-3951

current topics in solid state physics

Wiley

The solid state physics

Wiley

The solid state physics

The solid state ph

2008. Volume 5, 12 issues. Print ISSN 1610-1634 • Online ISSN 1610-1642

1500 citations of articles from 2004/05 (according to ISI Web of Science)

ISI Impact Factor (2006): 1.221

> www.pss-a.com

Special Issues in 2008

- Photonic crystals
- Organic field effect transistors
- Transparent electronics

> www.pss-b.com

ISI Impact Factor (2006): 0.967

Special Issues in 2008

- Computational nano-photonics
- Quantum Hall systems
- Silicon carbide

> www.pss-c.com

Special Issues in 2008

- II-VI semiconductors
- Advanced magnetic materials and applications
- Novel gain materials and devices

NEW Launched in 2007

2008. Volume 2, 6 issues. Print ISSN 1862-6254 • Online ISSN 1862-6270

> pss RRL will receive its first ISI Impact Factor in 2009

> www.pss-rapid.com

The fastest peer-reviewed publication medium in solid state physics



pss RRL offers extremely fast publication times: less than 14 days from submission to online publication and highest quality standards by thorough peer-review.

Don't miss the opportunity to receive complimentary online access to pss RRL throughout 2008. This special service is available to all institutions. Ask your librarian to register at

www.interscience.wiley.com/newjournals





For subscription details or to order a sample copy please contact Wiley Customer Service:

cs-journals@wiley.com (North and South America) service@wiley-vch.de (Germany / Austria / Switzerland) cs-journals@wiley.co.uk (All other regions)

Nanotube optics, Raman

8:30 – 9:30	T. Heinz, US Recent Advances in Understanding the Nature and Dynamics of Optically Excited States in Carbon Nanotubes
9:30 - 10:00	A. Hartschuh, DE
	Exciton Dynamics, Localization and Transfer in Single Car-
	bon Nanotubes
10:00 - 10:30	Coffee break
10:30 – 11:00	J. Lefebvre, CA
	Excitonic imaging spectroscopy of individual single-walled
	$carbon\ nanotubes$
11:00 – 11:30	R. Vogelgesang, DE
	Plasmonic nanostructures in aperture-less scanning near field optical microscopy (aSNOM)
11:30 – 12:00	F. Mauri, FR
	Probing the doping in metallic and semiconducting carbon
	nanotubes by Raman
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	R. Rhao, US
	Anharmonic Phonon Lifetimes in Carbon Nanotubes
19:00 – 19:30	A. G. Souza Filho, BR
	Electronic and vibrational properties of doped carbon nano-
19:30 – 20:00	tubes F. Simon, HU
13.50 20.00	Recent advances in the magnetic resonance studies of carbon
	nanotubes
20:00 - 20:30	K. Kamaras, HU
	Wide-range optical spectra of carbon nanotubes: a compara-

 $tive\ study$

Sunday, March 2

Recent Advances in Understanding the Nature and Dynamics of Optically Excited States in Carbon Nanotubes

Tony F Heinz

Departments of Physics and Electrical Engineering, Columbia University New York, NY 10027, USA

In this paper we present recent progress in elucidating the character and dynamics of optically excited states in single-walled carbon nanotubes. Two of the experimental frontiers in the optical spectroscopy of carbon nanotubes concern probing ultrafast dynamics and measurements at the individual nanotube level. After a review of the basic properties of the optical transitions in carbon nanotubes, we highlight progress in each of these directions.

The dynamical properties of carbon nanotubes are of considerable fundamental interest, as they relate to the basic interactions in the material, such as electron-electron, electron-phonon, and phonon-phonon couplings. While significant experimental work has addressed the rapid relaxation of electronic excitations, the decay the nonequilibrium phonon populations has not been probed directly. We describe how ultrafast optical techniques (time-resolved Raman scattering) can provide a direct measurement of the lifetime of optical phonons against anharmonic decay. These results relate to the role of non-equilibrium phonon distributions in current-carrying nanotubes.

Optical spectroscopy of individual single-walled carbon nanotubes is possible using both inelastic (Raman and fluorescence) and elastic (Rayleigh) light scattering techniques. We describe how the latter method allows one to probe in detail the influence of perturbations of the external environment on nanotubes of defined chiral index. The effect of strain and of the external dielectric environment, both observed in investigations by many groups, can be examined with considerable precision by single nanotube spectroscopy. In particular, we demonstrate the controlled modification of the nanotube band structure in space through a corresponding change of the external dielectric environment.

A detailed study of the lineshape of electronic transitions of individual nanotubes also provides new insights. While the excitonic nature of optical transitions in semi-conducting nanotubes has been established, significant electron-hole correlations in metallic nanotubes have also recently been predicted. Measurement of the lineshape of an isolated, individual metallic nanotube reveals a strong excitonic character to the transition, despite the expected effect of the screening provided by the free electrons.

Research results discussed in this paper involve extensive collaborations with the groups of Profs. Jim Hone, Louis Brus, and Stephen OBrien at Columbia University and with Prof. Feng Wang and his collaborators at UC Berkeley.

Exciton Dynamics, Localization and Transfer in Single Carbon Nanotubes

<u>Achim Hartschuh</u>¹ Huihong Qian¹ Carsten Georgi¹ Hayk Harutyunyan¹ Tobias Gokus¹ Mark C. Hersam² Frank Hennrich³ Lukas Novotny⁴

- ¹LMU Muenchen and CeNS, Muenchen
- ²Northwestern University, Evanston, Illinois
- ³Forschungszentrum Karlsruhe, Institut fuer Nanotechnologie, Karlsruhe
- ⁴University of Rochester, Rochester, New York

Optical excitation of nanotubes generates excitons that determine all light-based applications. We studied the decay dynamics, localization and transfer of excitons in single semiconducting nanotubes deposited on substrates using two complementary optical techniques. Exciton decay was monitored by time-resolved photoluminescence (PL) spectroscopy on a picosecond timescale. At room temperature the decay was found to be mono-exponential with lifetimes varying from 1 ps to 40 ps for nanotubes of the same chirality (n,m) [1]. To clarify the origin of the lifetime variations we studied the effects of the nanotube ends and the nanotube environment

Near-field PL and Raman imaging with a spatial resolution better than 15 nm was used to visualize the spatial extent of luminescent states along carbon nanotubes and to correlate electronic and structural properties [2,3]. The PL intensity was found to decrease towards the nanotube ends on a length scale of few 10 nm probably caused by efficient non-radiative recombination at localized end states [4]. Inter-nanotube energy transfer was studied for different pairs of semiconducting nanotubes forming bundles and crossings. PL from large bandgap nanotubes was observed with unexpectedly high intensities varying spatially along the nanotubes due to distance dependent transfer efficiencies. Efficient transfer is found to be limited however to a few nanometres because of competing fast non-radiative relaxation and can be explained in terms of electromagnetic near-field coupling.

- 1 A. Hagen et al, Phys. Rev. Lett. 95, 197401 (2005).
- 2 A. Hartschuh et al, Nano Lett. 5, 2310 (2005).
- 3 N. Anderson et al, Nano Lett. 7, 577 (2007).
- 4 P. Kim et al, Phys. Rev. Lett. 82, 1225 (1999).

Excitonic imaging spectroscopy of individual single-walled carbon nanotubes

Jacques Lefebvre¹ David G. Austing¹ Paul Finnie¹

 $\overline{^1\mathrm{Institute}}$ for Microstructural Sciences, National Research Council, Ottawa, ON, Canada, K1A 0R6

I will give a brief overview of some of the activities within our group related to carbon nanotubes, from synthesis with in situ optical characterization to fundamental studies related to optical and electronic properties. I will then discuss in detail the photoluminescence (PL) from individual semiconducting SWNTs grown free standing on patterned substrates.[1] We have demonstrated over the years that this type of sample is very well suited for fundamental studies of SWNT PL as interaction between the SWNT and its surrounding environment is minimized. More recently, we have used the bright PL signal to image SWNTs and to spatially resolve the emission from long nanotubes. PL imaging allowed for an estimate of the PL quantum yield to be around 10 %,[2] a value recently realized for nanotubes in solution, and an encouraging result from the point of view of possible applications. In addition, by acquiring PL images at different wavelengths of the laser, PL excitation (PLE) profiles have been obtained from individual nanotubes. By further controlling the polarization of the incident light with respect to the tube axis, polarized PLE (PPLE) profiles, both longitudinal and transverse have been obtained. In such experiments, the E_{12} transverse exciton with its (n,m) dependence and resulting family pattern was clearly identified.[3] Furthermore, for polarization along the nanotube axis, additional resonances have also been identified and are assigned to excited states of the E_{11} exciton, with their (n,m) dependence revealed. Data from new experiments which help to confirm and further extend the assignment of these spectral features will be presented.

- 1 J. Lefebvre, Y. Homma, and P. Finnie, Phys. Rev. Lett. **90**, 217401 (2003)
- 2 J. Lefebvre, D. G. Austing, J. Bond, and P. Finnie, Nano Letters 6, 1603 (2006)
- 3 J. Lefebvre, and P. Finnie, Phys. Rev. Lett. 98, 167406 (2007)

Plasmonic nanostructures in aperture-less scanning near field optical microscopy (aSNOM)

Ralf Vogelgesang¹ Jens Dorfmüller¹ Klaus Kern¹

¹Nanoscale Science, Abteilung Kern, Max Planck Institut für Festkörperforschung, Stuttgart

We review briefly the state-of-the-art in sub-wavelength optical microscopy. After an introduction to the essential aspects of scanning near field optical microscopy – in theory and implementation – we show how the cross-polarization scheme does afford us with an elegant method to map near fields of plasmonic eigenmodes and other optical phenomena. We conclude with recent examples that beautifully demonstrate the capabilities of this approach in studying optical properties of nanoscale structures.

11:30

Probing the doping in metallic and semiconducting carbon nanotubes by

 $\underline{F.~Mauri}^1$ A.M. Saitta 1 M. Lazzeri 1 N. Caudal 1 A. Das 2 A. K. Sood 2 A. Govindaraj 3 C. N. Rao 3

¹IMPMC, Universite Pierre et Marie Curie - Paris 6, Paris

² Department of Physics, Indian Institute of Science, Bangalore, India

³Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

In two recent works, we have shown theoretically that the Raman G bands of both metallic [1] and semiconducting [2] nanotubes are strongly affected by charge doping. In metallic nanotubes the G⁻ band exhibits a large increase in the Raman frequency, accompanied by a substantial decrease of its linewidth for both electron and hole doping, (the G⁺ band being unaffected). In semiconducting nanotubes, the G⁻ and G⁺ bands stiffen for both electron and hole doping (the G⁻ band being the most sensitive). Interestingly, the correct description of these phenomena requires the inclusion in the calculation of non-adiabatic effects beyond the Born-Oppenheimer approximation. The predicted behaviour is confirmed by Raman measurements combined with in-situ transport measurements on an ensemble of carbon nanotubes [2]. The source-drain conductivity is used to monitor the position of the Fermi level that is modified by electrochemical gating of the nanotubes with a solid polymer electrolyte. Similar experimental results were also obtained by two other groups [3,4]. In these works the Raman measurements were performed on individual tubes, but the shift of the Fermi energy with the Gate voltage was considered as a fitting parameter, i.e. it was not determined by transport data. Given the strong dependence of the Raman G bands on the Fermi energy, Raman spectroscopy can be used as an accurate measure of the doping of both metallic and semiconducting nanotubes, with important technological implications for nano electronics.

- 1 N. Caudal, A. M. Saitta, M. Lazzeri, F. Mauri, Phys. Rev. B 75, 115423 (2007)
- 2 A. Das, A. K. Sood, A. Govindaraj, A. M. Saitta, M. Lazzeri, F. Mauri, C. N. Rao, Phys. Rev. Lett. 99, 136803 (2007)
- 3 H. Farhat, H. Son, Ge. G Samsonidze, S. Reich, M. S. Dresselhaus, J. Kong, Phys. Rev. Lett. 99, 145506 (2007)
- 4 J. C. Tsang, M. Freitag, V. Perebeinos, J. Liu, Ph. Avouris, Nature Nanotechnology 2, 725 (2007)

Sunday, March 2

NT optics, Raman

NT optics, Raman

Sunday, March 2

Anharmonic Phonon Lifetimes in Carbon Nanotubes

 $\underline{\rm RAHUL~RAO^1}$ JOSE MENENDEZ² CHRISTIAN POWELEIT² APPARAO M $\rm RAO^1$

¹CLEMSON UNIVERSITY, CLEMSON

²ARIZONA STATE UNIVERSITY, TEMPE

High resolution Raman spectroscopy is applied to suspended single walled carbon nanotubes (SWNTs)to elucidate the puzzling differences in the lifetime of the radial breathing mode (RBM) obtained from different experimental techniques. Whereas recent tunneling experiments suggest a room temperature RBM lifetime as long as 10 ns, previous Raman experiments yield lifetimes shorter than 2 ps. The lifetimes obtained in this study are longer than 5 ps, a significant step in the direction of the tunneling results. We argue that the remaining discrepancy is due to the existence of phonon decay bottlenecks caused by the one dimensional nature of nanotubes. Numerical simulations of the RBM decay show that it is possible to reconcile the short lifetimes measured spectroscopically with the long lifetimes obtained in tunneling experiments.

19:00

Electronic and vibrational properties of doped carbon nanotubes

<u>Antonio G Souza Filho</u>¹ Eduardo B Barros¹ Mauricio Terrones² Oscar E D Rodrigues³ Vincent Meunier⁴ Morinobu Endo⁵ Y A Kim⁵ Hiroyuki Muramatsu⁵ Mildred S Dresselhaus⁶

- ¹Department of Physics, Universidade Federal do Ceara, Fortaleza
- ²Advanced Materials Department, IPICyT, San Luis Potosi, SLP, Mexico
- ³Centro Universitario Franciscano, Santa Maria, RS-Brazil
- ⁴Oak Ridge National Laboratory, USA
- ⁵Faculty of Engineering, Shinshu University, Nagano, Japan
- $^6\mathrm{Department}$ of Physics and Department of Electrical Engineering and Computer Science, MIT, MA USA

In this talk we present resonant Raman spectroscopy of doped carbon nanotubes. Emphasis is given to the use of this technique for studying functionalized carbon nanotubes obtained through chemical functionalization. We show how the different functionalization process can be used, for example, to tailor the electronic properties of the nanotubes such as a selective doping of the inner and outer shell of a double-walled carbon nanotube. The adsorption of bromine and sulfuric acid on double wall carbon nanotubes are discussed. We also discuss the properties of a new class of Selenium coated single wall carbon nanotubes.

References

- 1. A. G. Souza Filho et al., Nano Letters 7, 2383-2388 (2007).
- 2. E. B. Barros et al., Phys. Rev. B **76**, 045425 (2007).

3. A. G. Souza Filho et al., Phys. Rev. B **73**, 235413 (2006).

19:30

Recent advances in the magnetic resonance studies of carbon nanotubes

<u>F. Simon</u>¹ H. Kuzmany² B. Nafradi³ L. Forró³ D. Quintavalle¹ S. Toth¹ B. Dora⁴ P. Wzietek⁵ H. Alloul⁵

Magnetic resonance (ESR, NMR) methods are powerful to study low energy excitations i.e. the vicinity of the Fermi surface. This potentially enables to study strongly correllated phenomena in SWCNTs such as the Tomonaga-Luttinger liquid (TLL) phase, the Peierls transition, or superconducting correlations. We review the previous NMR results on ¹³C enriched nanotubes which support the observation of a gapped TLL state. Recent efforts to study the tube diameter dependence of the TLL ground state are described. In another approach, we encapsulate magnetic fullerenes and also non-covalently functionalize the tubes with spin-label molecules. ESR studies on these local paramagnetic probes show a uniform metallic behavior in the tubes down to 20 K.

20:00

Wide-range optical spectra of carbon nanotubes: a comparative study

<u>Katalin Kamaras</u>¹ Aron Pekker¹ Mark Bruckner¹ Ferenc Borondics¹ Mikhail E. It-kis² Robert C. Haddon² Andrew G. Rinzler³ David B. Tanner³ Yongqiang Tan⁴ Daniel E. Resasco⁴

We have studied the optical spectra of transparent carbon nanotube films made from various types of nanotubes: HiPCo, arc, laser and CoMoCat SWNTs, as well as double- and multiwall tubes. Comparing the optical conductivity calculated from transmission, estimates can be given on the metallic/semiconducting ratio in these films, as well as on the transparency window, the most important feature in applications. We find that while arc discharge and laser-ablated materials combine metallic dc conductivity with high transparency in the mid- and near infrared range, HiPCO and CoMoCat tubes exhibit a much lower metallic content and therefore lower conductivity. However, small-gap ($\sim 10 \text{ meV}$) tubes are present in the latter

¹Institute of Physics, Budapest University of Technology, Budapest

²Fakultät für Physik, Universität Wien, Strudlhofgasse 4, A-1090 Wien, Austria

 $^{^3}$ Institute of Physics of Complex Matter, FBS Swiss Federal Institute of Technology (EPFL), CH-1015 Lausanne, Switzerland

 ⁴Max-Planck-Institut für Physik komplexer Systeme, D-01187, Dresden, Germany
 ⁵Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France

¹Research Institute for Solid State Physics and Optics, Budapest, Hungary

²University of California, Riverside, CA, U.S.A.

³University of Florida, Gainesville, FL, U.S.A.

⁴University of Oklahoma, Norman, OK, U.S.A.

type of nanotubes as well. The window of transparency can be tuned by doping or by de-doping acid-purified samples.

Supported by the European Commission NEURONANO FP6 grant (NMP4-CT-2006-031847). Work at Florida supported by the NSF, DMR-0305043, and the DOE, DE-AI02-03ER46070.

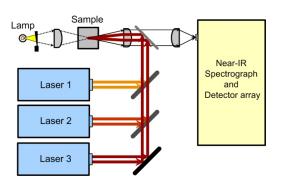
NT optics, Raman

Sunday, March 2

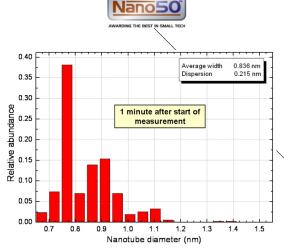
The NS1 NanoSpectralyzer

Automatic Fluorimetric Analysis of SWNTs

- Rapid near-IR fluorescence and absorption spectrometry
- ▶ High sensitivity
- ► Three lasers, compact design
- ➤ Small sample volumes
- ➤ Sophisticated, versatile software
- Automatic display of (n,m) distributions in seconds
- ➤ Turn-key system operation
- Support from pioneering nanotube spectroscopists
- Generous software updates reflect new research findings









in Europe, contact LOT-Oriel (schluetter@lot-oriel.de) Applied NanoFluorescence, LLC 3701 Kirby Drive, Suite 994 Houston, TX 77098 USA 713-521-1450 (voice / fax)

> info@appliednanofluorescence.com www.appliednanofluorescence.com

Graphene/Molecular electronics

8:30 – 9:00	S. G. Louie, US Novel Electronic and Optical Properties of Graphene and Graphene Nanoribbon
9:00 - 9:30	A. Lanzara, US
9:30 – 10:00	Quasiparticle dynamics in epitaxial graphene films A. Grüneis, DE Unravelling the electronic structure of intercalated graphite: a key to graphene and SWCNTs
10:00 – 10:30	Coffee break
10:30 – 11:00	B. Huard, US Potential barriers in graphene
11:00 – 11:30	S. Ilani, US Observation of Spin-Orbit Coupling in Clean Carbon Nano- tubes
11:30 – 12:00	K. Tsukagoshi, JP Gate control of conduction of thin graphite film
12:00 - 17:00 17:00 - 18:30	Mini Workshops Dinner
18:30 – 19:00	C. Jozsa, NL Graphene spintronics
19:00 – 19:30	A. J. R. da Silva, BR Ab initio design of reallistic nanotube sensors
19:30 – 20:00	T. González, CH Molecular junctions formed by break-junction techniques: electrical conductance determination at a single-molecule scale
20:00 – 20:30	V. Falko, UK Optics of electric flows in graphene

Monday, March 3

Novel Electronic and Optical Properties of Graphene and Graphene Nanoribbons

Steven G Louie

Physics Department, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory

In this talk, I discuss some recent theoretical results we obtained on the electronic and optical properties of graphene and graphene nanoribbons. These carbon nanostructures exhibit a number of unexpected behaviors. Our results on nanoribbons of different widths show that both armchair-edged graphene nanoribbons (AGNRs) and zigzag-edged graphene nanoribbons (ZGNRs) are semiconductors[1]. As in the case of nanotubes, self-energy[2] and excitonic[3] effects are dominant in the optical properties of these nanoribbons. The ZGNRs moreover are predicted to be half-metals under a sufficiently strong transverse electric field.[4] Theory further shows that, owing to the chiral nature of the electronic states, the dynamics of carriers (the 2D massless Dirac fermions) in graphene exhibits highly anomalous anisotropy when graphene is under an external periodic potential.[5] The physics behind these unusual behaviors is discussed.

- 1 Y.-W. Son, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 97, 216803 (2006).
- 2 L. Yang, C. H. Park, Y.-W. Son, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 99, 186801 (2007).
- 3 L. Yang, M. L. Cohen, and S. G. Louie, Nano Letters 7, 3112 (2007).
- 4 Y.-W. Son, M. L. Cohen, and S. G. Louie, Nature 444, 347 (2006).
- 5 C. H. Park, L. Yang, Y.-W. Son, M. L. Cohen, and S. G. Louie, Nature Physics (2008), in press.

9:00

Quasiparticle dynamics in epitaxial graphene films

<u>Alessandra Lanzara</u>

Department of Physics, University of California, Berkeley, USA Lawrence Berkeley National Laboratory, Berkeley, California

The electronic structure of single and bilayer graphene films is studied by high resolution angle resolved photoemission spectroscopy. The evolution of the band structure and many body interactions is studied as a function of sample thickness. By monitoring the film growth with low energy electron microscopy (LEEM) sample with different domain size are grown. The effect of confinement on the band structure is discussed.

Unravelling the electronic structure of intercalated graphite: a key to graphene and single-wall carbon nanotubes

<u>A. Grüneis</u>¹ C. Attaccalite² A. Rubio² S.L. Molodtsov³ D. Vyalikh³ W. Eberhardt⁴ J. Fink⁴ T. Pichler⁵

¹IFW Dresden, P.O. Box 270116, D- 01171 Dresden, Germany

 2 European Theoretical Spectroscopy Facility, Department of Material Physics, University of the Basque Country, 20018 San Sebastian, Spain

³Institut fuer Festkörperphysik, TU Dresden, Mommsenstrasse 13, D-01069 Dresden, Germany

⁴BESSY II, Albert-Einstein Strasse 15, 12489 Berlin, Germany

⁵Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria

Understanding the unique low energy electronic structure of carbon systems is the key for their peculiar properties [1]. In this contribution we show how to unravel electronic correlations in pristine and intercalated (stage I, II and III) graphite single crystals from the quasi particle dispersion of the valence band electrons using a combined angle resolved photoemission and theoretical approach. We report the full three-dimensional renormalized band dispersion and the strength and angular dependence of the electron-electron and electron-phonon interactions as a function of doping. We also emphasize on the effect of different inter layer couplings in intercalation compounds and the implications on the band structure. We will show that these results enable us to accurately determine key properties, such as Fermi velocities, effective masses and electron-electron and electron-phonon coupling constants in graphite and weakly coupled graphene layers without substrate interaction. We highlight the implications of our results for the understanding of transport, superconductivity and the resonance Raman effect in a wide range of sp2 hybridised carbon systems such as graphene, graphite and single wall carbon nanotubes.

1 A. Grüneis et al. Phys. Rev. Lett. 100, 037601 (2008).

10:30

Potential barriers in graphene

Benjamin Huard

Stanford University, Stanford

The peculiar nature of electron scattering in graphene is among many exciting theoretical predictions for the physical properties of this material. To investigate electron scattering properties in a graphene plane, we have created a gate-tunable potential barrier within a single-layer graphene sheet. We report measurements of electrical transport across this structure as the tunable barrier potential is swept through a range of heights. When the barrier is sufficiently strong to form a bipolar

junction (n-p-n or p-n-p) within the graphene sheet, the resistance across the barrier sharply increases. We compare these results to predictions for both diffusive and ballistic transport, as the barrier rises on a length scale comparable to the mean free path.

11:00

Observation of Spin-Orbit Coupling in Clean Carbon Nanotubes

Shahal Ilani¹ Ferdinand Kuemmeth¹ Dan C. Ralph¹ Paul L. Mceuen¹ Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca NY 14853

The electronic states in defect-free carbon nanotubes are widely believed to be four-fold degenerate, due to independent spin and orbital symmetries, and also to possess electron-hole symmetry. We report measurements demonstrating that in clean nanotubes the spin and orbital motion of electrons are coupled, thereby breaking all of these symmetries. This spin-orbit coupling is directly observed as a splitting of the four-fold degeneracy of a single electron in an ultra-clean quantum dot. Application of a parallel magnetic field reveals that the coupling favours parallel alignment of the orbital and spin magnetic moments for electrons and anti-parallel alignment for holes. We further show that spin-orbit coupling determines the filling order in the many-electron ground states, in a way different than that expected from electron-electron interactions. At low magnetic fields we find that the two-electron ground state is neither a spin-triplet nor a spin-singlet, but a Slater determinant in which the spin and orbital wavefunction are entangled. Our findings have important implications for spintronics applications in nanotubes and provide a mechanism for all-electrical control of spins in this system.

11:30

Gate control of conduction of thin graphite film

Kazuhito Tsukagoshi RIKEN, AIST, JST-CREST, Hirosawa

We present fundamental researches on gating control in thin graphite film. Observed resistance in the gate-voltage change applied by back-gate shows ambipolar behaviour based on clear carrier polarity change. A front gate, which was directly formed on the surface of the graphite film, also changes the resistance of the thin graphite film. By operating the two gates in the thin graphite film with various film-thickness, we could find that the screening length of the electric field from the gate electrode could be experimentally estimated. The estimated length was 1.2 nm, corresponding to the a few layers in the graphite. We also measured proximity superconducting current in the thin graphite film with superconducting electrodes. The gating effect of the proximity current can be reasonably explained in consideration with the screening effect of the gate electric field. Furthermore,

in a graphene ribbon, the gate electric field easily penetrate the thin ribbon and transfer a structural roughness of the film as the electrical potential fluctuation in the conduction channel. As a result, multiple Coulomb islands were formed, and the Coulomb blockade oscillations were observed.

Graphene/Molecular electronics

Monday, March 3

Graphene spintronics

 $\underline{\text{Csaba Jozsa}^1}$ Nikolaos Tombros^1 Mihaita Popinciuc^1 Harry T. Jonkman^1 Bart J. van Wees^1

¹Zernike Institute for Advanced Materials, University of Groningen, The Netherlands,

We report the observation of spin transport as well as spin precession over micrometer long distances using graphene based field effect transistors. Our experiments were done on four terminal non-local contact geometries using ferromagnetic cobalt electrodes. Clear bipolar (changing from positive to negative sign) spin signals were observed, which reflect the magnetization direction of all 4 electrodes, indicating that spin coherence extends underneath all 4 contacts. From the dependence of the spin signal on electrode spacing we deduce that the spin relaxation length is in the range of 1.5 to 2 micrometer. These values are confirmed by spin precession measurements (Hanle effect). We find good agreement with the diffusion constants derived from conductivity measurements at the Dirac point, or at high densities. No significant changes in the spin signals occur between 4.2K, 77K and room temperature. The spin polarization of the ferromagnetic contacts is estimated to be around 10%. Finally, we will show our latest results concerning the drift of the injected spins under the influence of an applied DC electric field and the drift-diffusion model we use to interpret these results.

19:00

Ab initio design of reallistic nanotube sensors

Antonio J. R. da Silva¹ A. R. Rocha¹ M. Rossi¹ A. Fazzio¹ Instituto de Fisica, Universidade de Sao Paulo, SP Brazil

The understanding of the electronic transport properties of nanoscopic devices present tantalizing possibilities. In particular it has been demonstrated that carbon nanotubes can be used as sensors for hazardous gases. Large scale computer simulations have an important role to play in predicting the transport properties of such systems. In order to do so one must take into account devices which are a few hundred nanometers in length and present defects randomly distributed along the structure. These defects act as binding sites for the molecules one wishes to detect. In this work we initially use density functional theory (DFT) to determine the most likely defects in highly nitrogen-doped carbon nanotubes, and to calculate the dissociation path of ammonia and hydrogen sulphide molecules onto these defects. Finally we use a combination of DFT and recursive Greens functions techniques to first assemble and then calculte the electronic transport properties of nanotubes up to 200 nm in length and with defects randomly distributed along the structure. We demonstrate that these nanotubes present relatively large resistance changes even at low coverages which leads to highly sensitive devices. The result is

a new paradigm in computer-aided sensor design, where one can simulate rellistic sensors.

19:30

Molecular junctions formed by break-junction techniques: electrical conductance determination at a single-molecule scale

 $\underline{\text{Teresa Gonz\'alez}^1}$ Roman Huber 1 Songmei Wu 1 Jan Brunner 1 Christian Schönenberger 1 Michel Calame 1

¹Institut für Physik, Basel Universität, Basel

Break-junction experiments appear as the most promising techniques for exploring the electrical transport properties of a single molecule. It is generally interpreted that a molecular junction forms when one or a few molecules covalently bond at their ends to two metallic tips, which are moving apart from each other. However, the variety of conductance values reported in the literature for a given molecule reflects the complexity of these molecular junctions.

In this work, we explore several simple molecules with the aim of learning the details of the molecular bridge formation. A mechanically controllable break junction technique has been used to explore the conductance of molecular junctions based on alkanedithiols, and several derivatives of oligo(phenylene elthynylene)s (OPEs) and oligo(phenylene vinylene)s (OPVs). All the experiments have been carried out at room temperature and in liquid environment.

20:00

Optics of electric flows in graphene

Vladimir Falko

Lancaster University, Lancaster, UK

Both monolayer and bilayer graphene are gapless semiconductors. Their electrostatic modulation can be used to generate single and multiple p-n junctions. We have shown [1] that p-n junctions in monolayer graphene are transparent for incident electrons. In particular, those electrons approaching the n-p interface in an almost perpendicular direction can cross it without reflection. Moreover, in graphene the transmission of charge through the n-p interface is quite similar to the refraction of electromagnetic waves at the interface where the refractive index inverts sign [2]. This is because the electron dispersion in the conduction and valence bands in graphene is such that so that, after an electron crosses the n-p interface, from the n- to p-side, its wave vector becomes directed opposite to its velocity. As a result, n-p junctions in graphene possess intriguing and very promising transport properties: a single straight p-n interface can focus electrons [3]. This situation is realised in the n-p junction with equal densities of carriers in the n- and p-regions. Also, we have shown that by varying the carrier density in, e.g., p-side of the junction the focus can be smeared into a pair of caustics meeting each other in a cusp, and

calculated the characteristic interference pattern of electron waves in the vicinity of the cusp. Using the idea of fine-tuned focusing of electron flow by the p-n interface, we propose to use n-p-n junction In a bipolar graphene-based transistor to create Veselago lens and focused beam splitters for electrons.

- 1 V. Cheianov and V.I. Falko Phys. Rev. Lett. 97, 226801 (2006).
- $2\,$ J. Pendry Nature 423, 22 (2003); J. Pendry Phys. Rev. Lett. 85, 3966 (2000).
- 3 V. Cheianov, V.I. Falko, B.L. Altshuler Science 315, 1252 (2007).

Graphene/Molecular electronics

Monday, March 3



Bruker Optics



Contact us for more details: www.brukeroptics.com

FT-IR

NT transport, Devices

20:00 - 21:00 Poster Session - TUE

8:30 – 9:30 9:30 – 10:00	JC. Charlier, BE Quantum Transport in Carbon Nanotubes M. Bockrath, US The One-Dimensional Wigner Crystal in Carbon Nanotubes
10:00 – 10:30	Coffee break
10:30 – 11:00	T. Fukushima, JP Soft Materials with Carbon-Rich Nanostructures
11:00 – 11:30	M. Freitag, US Photovoltage microscopy and Raman spectroscopy of individual carbon nanotubes
11:30 – 12:00	Y. Nakayama, JP Plastic Bending Deformation of Carbon Nanotubes
12:00 - 17:00 17:00 - 18:30	Mini Workshops Dinner
18:30 – 19:00	A. Bachtold, ES Nanotube ElectroMechanics
19:00 – 19:30	C. Hierold, CH SWNT Functional Structures in Sensors
19:30 – 20:00	B. Yakobson, US Nanotubes in global warming: From dynamic topology in superplasticity to hyperthermia in cancer treatment

Tuesday, March $4\,$

Quantum Transport in Carbon Nanotubes

Jean-Christophe Charlier

Université Catholique de Louvain Unité de Physico-Chimie et de Physique des Matériaux (PCPM), Place Croix du Sud 1, B-1348 Louvain-la-Neuve, Belgium

Their unusual electronic and structural physical properties promote carbon nanotubes as promising candidates for a wide range of nanoscience and nanotechnology applications. Not only can nanotubes be metallic, but they are mechanically very stable and strong, and their carrier mobility is equivalent to that of good metals, suggesting that they would make ideal interconnects in nanosized devices. Further, the intrinsic semiconducting character of other tubes, as controlled by their topology, allows us to build logic devices at the nanometer scale, as already demonstrated in many laboratories.

The tremendous importance of the transport properties of nanotubes [1], both from a fundamental and technological point of view, justifies wealth of work and theories developed to deal with 1D systems involving a confined electron gas. The purpose of the present talk is to define the electronic and transport properties of nanotubes in relation with their atomic structures. Since quantum effects are prominent in nanotube physics, the electronic quantum transport has been investigated using both the Landauer-Buttiker and the Kubo-Greenwood formalisms, allowing to extract generic properties such as quantum conductance, conduction mechanisms, mean-free-paths... Within both frameworks, the well-known ballistic properties of armchair metallic nanotubes have been reproduced. However, defects, doping and chemical functionalisation can alter this ideal situation. For example, even a small amount of boron or nitrogen dopants can drastically modify the electronic transport properties of the tube, which is certainly a key effect for future nanoelectronics [2]. The chemical sensitivity of the electronic transport in carbon nanotubes under the physisorption of molecular species [3] or covalent functionalisation is also an important issue as for example in sensing applications.

Like in most materials, the presence of defects in carbon nanotube has been demonstrated experimentally. These defects may take different forms: vacancy, bivacancy, "Stone-Wales" defect, 5/7 pair, atom in substitution, ... and are known to modify the electronic properties of carbon nanotubes [4]. It is crucial to understand the properties of these defects in order to conquer their detrimental effects, but also because controlled defect introduction may be used to tune nanotube properties in a desired direction. Consequently, the modifications induced by those defects in the electronic properties of the carbon hexagonal network have been investigated using first-principles calculations. Computed constant-current STM images of these defects have been calculated within a tight-binding approach in order to facilitate the interpretation of STM images of defected carbon nanostructures. At last, as these defects should also play a key role in the chemical reactivity of carbon nanotubes, the study of the modulation of the conductance due to specific molecules adsorbed at the defected nanotube surface will be presented.

- 1. Electronic and transport properties of nanotubes, J.-C. Charlier, X. Blase, and
- S. Roche, Reviews of Modern Physics 79, 677-732 (2007)
- 2. Mesoscopic transport in chemically doped carbon nanotubes, S. Latil, S. Roche,
- D. Mayou, and J.-C. Charlier, Physical Review Letters 92, 256805 (2004)
- 3. Electronic transport in carbon nanotubes with random coverage of physisorbed molecules, S. Latil, S. Roche, and J.-C. Charlier, Nano Letters 5, 2216-2219 (2005)
- 4. Scanning tunneling microscopy fingerprints of point defects in graphene: a theoretical prediction, H. Amara, S. Latil, V. Meunier, Ph. Lambin, and J.-C. Charlier, Physical Review B 76, 115423 (2007)

The One-Dimensional Wigner Crystal in Carbon Nanotubes

Marc Bockrath

California Institute of Technology, Pasadena

in the absence of disorder, a dilute system of carriers interacting through long-range Coulomb forces has been predicted to form a periodic solid called the Wigner crystal. We demonstrate using low-temperature single-electron transport spectroscopy that a low-density hole system in low-disorder carbon nanotubes with a band gap is a realization of the one-dimensional (1D) Wigner crystal. The two inequivalent Dirac points defining the nanotubes' band structure yield an isospin degree of freedom so that the holes act as a spin and isospin chain. We find three distinct regimes as the applied axial magnetic field and carrier density are varied: a fully spin and isospin polarized regime, an isospin-polarized, spin antiferromagnetically-ordered regime, and an unpolarized regime.

These regimes arise from a competition between exchange and magnetic energy in the spin and isospin chain. We account for our observations quantitatively using the gapped Luttinger-liquid model of Levitov and Tsvelik. We also observe an abrupt disappearance of the Kondo effect versus magnetic field, which we attribute to the interplay between the spin and isospin degrees of freedom that yields larger spin states than would be predicted using a shell-filling picture. Our observation provides a clear demonstration of the effect of electronic correlations on the properties of 1D systems and provides a clean platform for testing theories of interacting electrons in low-dimensional materials.

Soft Materials with Carbon-Rich Nanostructures

<u>Takanori Fukushima</u> RIKEN, JST ERATO-SORST, U. Tokyo

Our recent studies on novel soft materials consisting of carbon-rich nanostructures will be described. For example, single-walled carbon nanotubes, when suspended in imidazolium ion-based ionic liquids and ground in an agate mortar, form physical gels, where heavily entangled bundles of carbon nanotubes are exfoliated to give highly dispersed fine bundles. By utilizing the gels, the first printable actuators that operate in air for a long time without any external electrolytes were developed. Furthermore, the use of polymerizable ionic liquids as the gelling media gave rise to the formation of electroconductive polymer/nanotube composites with enhanced mechanical properties. The lecture will also include the synthesis of new carbon-rich nanotubes via self-assembly of Gemini-shaped hexabenzocoronene amphiphiles. The walls of the nanotubes consist of pi-stacked hexabenzocoronene units, providing charge-carrier transport pathways. The use of hexabenzocoronene derivatives with functional groups results in the formation of nanotubes with various interesting properties.

11:00

Photovoltage microscopy and Raman spectroscopy of individual carbon nanotubes

Marcus Freitag

T.J. Watson Research Center, IBM, Yorktown Heights, NY

In this talk, we describe microscopic measurements of important device parameters of carbon nanotube field-effect transistors. The Schottky barrier heights and depletion widths are extracted from photovoltage images acquired under a scanned focused laser spot. In fact, the entire band bending in ambipolar transistors can be observed as it changes from p-type through intrinsic to n-type, during a gate voltage sweep. Single defects are also seen in these images. In either n-type or p-type on-states, the band bending changes only weakly because of the high density of states at the band edge in one-dimensional materials. However, we find by Raman spectroscopy that the energies of the G-band phonons renormalize in a predictable way, allowing the extraction of the charge density and thus the capacitance of the device. The phonon renormalization is present even though related effects, such as Kohn anomalies or charge density waves, are absent in semiconducting materials. In metallic carbon nanotubes, we find in agreement with previous measurements on graphene that both energy and linewidth of the G-band phonons change upon doping. This work was done in collaboration with James Tsang, Vasili Perebeinos, Ageeth Bol, Dongning Yuan, Jie Liu, and Phaedon Avouris.

Plastic Bending Deformation of Carbon Nanotubes

Yoshikazu Nakayama

Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

We have investigated two types of current-induced plastic bending deformation of carbon nanotubes (CNTs). The first one (mode I) is the transformation from elastic bend without buckling to plastic bend by applying a current [1]. The second one (mode II) is from elastic bend with buckling to plastic bend [2].

For mode I the onset of circumferential current density is quite low as compared with that for the sublimation of CNTs and decreases with increasing the diameter. The resultant bending angles are from 20 to 30 degrees. We have discovered the one-way shape memory effect (SME) that the original straight position of a CNT with an artificially induced plastic bend is recovered by applying a high current nearly equivalent to the value causing sublimation [3]. We also found that applying such high current to the elastic bend with buckling causes the plastic bend with a larger bending angle. This is mode II of the plastic deformation.

The computer simulations based on the analysis using minimum energy path calculation with a bond-order potential have revealed that the plastic deformation of mode I is only thermodynamically favorable above a threshold curvature [4]. The initiation is 5-7-7-5 defect nucleation with ca. 5 eV at the maximum strain region, and then two 5-7 pairs are separated from the defect and glide toward a position with a minimum formation energy to form the plastic bend.

The theoretical work on the plastic bending of (5,5)/(10,10) double-walled CNT revealed that only the outer tube is plastically deformed at a lower applied bending curvature and both the inner and outer tubes at a higher bending curvature [5]. The outer tube is tougher for the plastic deformation than the single-walled CNT with the same diameter due to tube-tube interactions. In contrast, the plastic deformation of the inner tube is not strongly affected by the presence of the outer tube.

The simulation on the SME clarified that the defect annihilation energy is negative in both single- and double-walled CNTs [5]. The thermal recovery of double-walled CNT is kinetically easier than that of single-walled CNT, because the 5-7 pair energy increases with its migration in the first several steps for single-walled CNT.

- 1 Y. Nakayama et al., Jpn. J. Appl. Phys. 44, L720 (2005).
- 2 H. Somada et al., Jpn. J. Appl. Phys. 46, L1055 (2007).
- 3 O. Suekane et al., Appl. Phys. Lett. 89, 183110 (2006).
- 4 H. Mori et al., Phys. Rev. B 74, 165418 (2006).
- 5 H. Mori et al., Phys. Rev. B 76, 165405 (2007).

NT transport, Devices

Tuesday, March 2

Nanotube ElectroMechanics

Adrian Bachtold
CIN2 Barcelona, Bellaterra

Carbon nanotubes are often recognized as the ultimate material for high-frequency mechanical resonators. For instance, nanotube resonator devices hold promise for ultralow mass detection or quantum electromechanical experiments. However, the detection of the mechanical vibrations remains very challenging. In this talk, I will present a novel detection method of nanotube vibrations, which is based on atomic force microscopy. This method enables the detection of the resonances up to 3.1 GHz with subnanometer resolution in vibration amplitude. Importantly, it allows the imaging of the mode-shape for the first eigenmodes.

I will also report on a new artificial nanofabricated motor in which one short nanotube moves relative to another coaxial nanotube. This motion is shown to consist of translation and/or rotation, depending on the atomic interaction between the nanotubes. The motion is actuated by imposing a thermal gradient along the device, allowing for sub-nanometer displacements. This is, to our knowledge, the first experimental demonstration of displacive actuation at the nanoscale by means of a thermal gradient.

19:00

SWNT Functional Structures in Sensors

<u>Christofer Hierold</u>¹ Thomas Helbling¹ Lukas Durrer¹ Cosmin Roman¹ ETH Zurich, Zurich

SWNT are considered excellent functional structures for sensors: outstanding electromechanical properties in semiconducting SWNTs, high surface to volume ratio and lowest mass for sensitive (bio)chemical sensors down to single molecule detection. This paper reports on concepts for carbon nanotube based sensors for mechanical and chemical quantities. We focus on single-walled carbon nanotubes as simple macro molecular functional structures with an option for integration in micro- and nanosystems or MEMS and NEMS. We present and discuss research results on CNT fabrication and integration, and electronic characterization, including signal-to-noise in SWNT-FET based structures and zero-level packaging by ALD alumina.

Nanotubes in global warming: From dynamic topology in superplasticity to hyperthermia in cancer treatment

Boris I. Yakobson

Department of Mechanical Engineering & Materials Science, Department of Chemistry, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, TX

Two phenomena involving carbon nanotubes (NT) will be discussed. One occurs at very high temperature near 2000 C. Another takes place upon relatively minor yet biologically significant warming by just 10-50 C.

Early considerations of dynamic topology of NT at high temperatures have predicted the possibility of plastic flow and quantized necking accompanied by the change of the electronic band gap. Past two years have brought spectacular experimental confirmations to those predictions, while also revealed new intriguing features of superplasticity. The glide of pentagon-heptagon defects and a particular type of their pseudo-climb, act concurrently to maintain the tube perfection, even in spite of great mass loss in sublimation [1]. Their dynamics disobey the Frank rule, showing fundamental difference of dislocation theory in non-Euclidean 2D lattice of NT [2] from the traditional 3D crystals.

Recently, our MDACC collaborators have discovered the ability of NT to heat up in a radiofrequency (RF) electromagnetic field, which can be used to locally induce hyperthermia to kill cancer cells and tumors [3]. One working hypothesis of RF-induced Joule heating emphasizes the role of large aspect ratio (length/diameter) and allows us to reconcile the high power deposition (up to $100,000~\mathrm{W/g}$ of NT) with very low NT concentrations (from 10^{-5}) in aqueous solution.

- 1 F. Ding, et al., Phys. Rev. Lett. 98, 075503 (2007); Nano Lett. 7, 681 (2007).
- 2 J. Huang, et al., Phys. Rev. Lett. 99, 175503 (2007); Phys. Rev. Lett. 100, 035503 (2008).
- 3 C. Gannon, P. Cherukuri, et al., Cancer 110, 2654 (2007).

NT transport, Devices

Tuesday, March 2

REORGANIZATION OF FULLERENE CLUSTERS IN THE SYSTEM C60/NMP/WATER AFTER ADDITION OF WATER

 $\underline{\rm V.L.~Aksenov}^1$ M. V. Avdeev 1 O.A. Kyzyma 2 T.V. Tropin 1 S.V. Snegir 3 M.V. Korobov 4 L. Rosta 5

¹Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Moscow Region, Russia

²Physical Faculty, Kyiv Taras Shevchenko National University, Kyiv, Ukraine

³Institute of surface chemistry, NAS of Ukraine, Kiev, Ukraine

⁴Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

⁵Research Institute for Solid State Physics and Optics, Budapest, Hungary

The clusterization of fullerene C60 in different nitrogen-containing solvents, as well as in their mixtures with water is connected with specific features of this class of solvents regarding the interaction with fullerenes. In the present work we analyze the effect of cluster decomposition in the system C60/N-methylpyrrolidone (NMP) after addition of water as observed by small-angle neutron scattering (SANS) and mass spectroscopy. It is shown that the characteristic size (more than 100 nm) in pure C60/NMP solution decreases after addition of water into the system. Mass spectra indicate that the decomposition of clusters in solutions occurs as a result of the monomer detachment. The observed mechanism explains the age effect of the initial C60/NMP solution on the cluster size in the system C60/NMP/water.

2

Irradiation induced increase of GeOx responsible for 3.2 eV emission at Ge nano-crystals a

-SiO2 interfaces

Antonino Alessi¹ Simonpietro Agnello¹ Franco Mario Gelardi¹ Roberto Boscaino¹ Department of Physical and Astronomical Sciences, University of Palermo, Palermo

Many investigations, about the generation processes of Ge nanocrystals (ncGe) in amorphous SiO_2 (aSiO_2), have shown that together with such structures there is an interface layer of substoichiometric Ge oxide: GeO_x, with x between 0 and 2. In such structured materials, together with ncGe, the presence of a photoluminescence band centred at 3.2 eV is often detected. This emission is attributed to an excitonic electron hole pair recombination process in the ncGe, but different studies have suggested that this emission activity is related to a recombination on defects of the GeO_x layer. The type of defects responsible of this luminescence is the twofold coordinated Ge, a Ge atom connected with two oxygens and with two electron forming a lone pair. Our data on 60Co gamma irradiated Ge doped aSiO_2 show the possibility to induce these centers in bulk samples. The induced defects concentration depends n Ge content, as expected, and are explained on the

basis of irradiation enhancement o substoichiometry. This suggests the possibility to probe the origin of the photoluminescence at ncGe aSiO_2 interfaces by increasing the concentration of twofold coordinated Ge and as a consequence of the 3.2 eV emission intensity.

3 Structural properties of carbon nanostructures under low temperature and

Vincent JOURDAIN Robert ALMAIRAC Rozenn LEPARC Jean Louis SAU-VAJOL Jean Louis BANTIGNIES LAURENT ALVAREZ Jonathan ROSE Lawrence T. SCOTT

¹LCVN, Unicersity Montpellier II, Montpellier, FRANCE

²MERKERT CHEMESTRY CENTER, Boston College, Chestnut Hill, Massachusetts, USA

We propose here a study of the structural evolutions of corannulene under high pressure and low temperature. Results obtained by Raman spectroscopy are presented.

4

A Method to Coat Sharpened Tungsten Wires with Multiwall Carbon Nanotubes for Enhanced Electrode Performance

Alberto Ansaldo¹ Siegmar Roth² Davide Ricci¹

Carbon Nanotubes (CNTs), thanks to their ability to provide an efficient path for charge transport, have been proposed in various occasions for electrochemical applications. Electrodes coated with CNTs improve their performance thanks both to the greatly increased exposed surface and to the reduced effective work function. While several experiments of CNTs deposited or grown onto planar metal electrodes have been reported, direct growth of Multiwall Carbon Nanotubes (MWCNTs) via Chemical Vapour Deposition (CVD) onto electrochemically sharpened Tungsten wires is, to our knowledge, a new result that we present in this work. To this end, a key issue has been the ability to coat with the CNT catalytic precursors the Tungsten wire up to its very apex. The tips have been dipped into a precursor ink containing Nickel nanoparticles and then placed in a reactor where MWCNTs have been grown directly using alcohol CVD at a temperature between 550 and 700°C. The morphology of the MWCNTs coatings depending on the catalyst precursor ink concentration and thermodynamic growth parameters is discussed. A comparison in the performance of pristine versus coated electrodes is performed and their electrochemical properties and applications are discussed.

¹Istituto Italiano di Tecnologia, Genova - Italy

²Max-Planck-Institut für Festkörperforschung, Stuttgart - Germany

Anomalous Structural Dependence of the Radial Breathing Mode in Single Wall Carbon Nanotubes

Stephen K. Doorn¹ Huihong Qian² Achim Hartschuh² Paulo T Araujo³ Ado Jorio³ Indhira O. Maciel³ Pedro B. Pesce³ Marcos A. Pimenta³ Simone S. Alexandre³ Helio Chacham³ Mathias Steiner⁴ Kenji Hata⁵

¹Chemistry Division, Los Alamos National Laboratory, Los Alamos, USA.

²Departament Chemie und Biochemie and CeNS, Ludwig-Maxmilians-Universitaet Muenchen, Germany.

³Departamento de Fisica-Instituto de Ciencias Exatas-ICEx, Universidade Federal de Minas Gerais-UFMG, Belo Horizonte, MG.

⁴IBM Research Division, T.J. Watson Research Center, Yorktown Heights, New York.

⁵Research Center for Advanced Carbon Materials, (AIST), Tusukuba, Japan.

Despite its importance, the structural dependence of the single wall carbon nanotube (SWNT) radial breathing mode frequencies (ω_{RBM}) is not established. Here resonant Raman scattering is used to determine the ω_{RBM} of SWNTs grown by the water assisted chemical vapor deposition method. We find an anomalous dependence of the ω_{RBM} versus tube diameter (d_t), as compared to tubes grown by other techniques. First, the ω_{RBM} are downshifted by an amount that increases, in modulus, with d_t . Second, the frequencies are well fitted by the relation $\omega_{RBM} = 227.0/d_t$, which agrees with the graphene sheet limit ($1/d_t \rightarrow 0$), in contrast with the relation $\omega_{RBM} = A/d_t + B$ that is obtained for tubes grown by other techniques. We propose possible extrinsic and intrinsic effects that may account for the observed anomalies.

6 New Phase of Polymeric C60: Double Chains via [2+2] Cycloaddition

Vasilii I. Artyukhov¹ Elena E. Belova¹ Leonid A. Chernozatonskii¹

¹Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, 119334 Russia

We report *ab initio* calculations of a new phase of polymeric C_{60} . This phase has recently been demonstrated to form from the O phase of polymeric C_{60} at high pressures (≈ 0.5 GPa) under laser or x-ray irradiation [R. Le Parc *et. al.*, *Chem. Phys. Lett.* 438, 63 (2007)]. We investigate the structural changes that polymeric C_{60} undergoes under such conditions. The transition to the new phase involves additional [2+2] cycloadditions between neighboring C_{60} chains of the O phase, forming double chains of C_{60} units along the [100] direction. The new phase is a semiconductor, like the original O phase, but with a smaller band gap.

Electronic and Optical properties of B-doped Single Wall Carbon Nanotubes

Paola Ayala¹ Thomas Pichler² Hans Kuzmany² Esko Kauppinen¹

¹Lab.of Physics and Center for New Materials, Helsinki University of Technology, Espoo, FINLAND

²Faculty of Physics, Universitaet Wien, Vienna, AUSTRIA

It is well known that one efficient method of tailoring the electronic properties of single wall carbon nanotubes is the chemical modification through incorporation of heteroatoms within the tube walls. In fact, an efficient doping can be achieved by substituting carbon by heteroatoms such as boron due to its chemical electronic configuration. Besides the experimental reports on the successful synthesis of boron doped carbon nanotubes (CNTs) with methods such as substitution reactions, arc discharge and laser ablation we reported recently a chemical vapor deposition method which involves exclusively the use of a pure liquid C/B feedstock. In the present contribution we show how the use of solely one feedstock of a constant vapor pressure facilitates a controlled growth of even morphology samples. Raman spectroscopy and TEM have revealed very low defect concentration concomitant with small nanotube bundles containing 5-8 tubes with a narrow diameter distribution. Regarding the incorporation profile of B within the tubes, a pioneering x-ray photoelectron spectroscopy analysis will be presented revealing unusual features in the peak positioning and shape according to B incorporation. An overall observation demonstrates a growth window for doped SWCNT with diameters ranging between 1 and 3 diameters between 770 and 1000C. Although, a multifrequency Raman analysis has proved that the tube diameter distribution remains constant notwithstanding the synthesis temperature, added to a narrow diameter distribution of small diameter tubes between 0.9 and 1.4nm. An analysis of the tube relative fraction of metallic tubes as well as the tube chiralities has been carried out based on the theoretical and experimental Kataura plots. Furthermore comparative fluorescence studies on the same samples will be presented.

Work supported by DFG and BCN-Nanotubes EU project.

8

Insitu growth of carbon nanotubes in thermogravimetric analyzer coupled to mass spectrometer

Alicja Bachmatiuk¹ Anna Steplewska¹ Ewa Borowiak-Palen¹ Ryszard J. Kalenczuk¹

Here we present the preliminary result on a novel experiment of the insitu growth of different carbon nanotubes in thermogravimetric analyzer coupled to mass spectrometer (TGA-MS). The system allows to analyze the changes in mass in TGA mode and the evolved gases during the process in MS mode. We believe that the

¹Szczecin University of Technology, Poland, Szczecin

detailed study of the process can lead to the better understanding of the process of the carbon nanotubes mechanism growth. The analysis of this phenomena will be supported by high resolution transmission electron microscope (HR-TEM) and resonance Raman spectroscopy.

9 NEXAFS study of nitrogen doping of carbon nanotubes

Jean-Louis Bantignies Laurent Alvarez Francois Lenormand Shaima Enouz $\overline{^1}$ Laboratoire des colloides verres et nanomateriaux, University of Montpellier 2, MONTPELLIER

²Institut de Physique et Chimie des Materiaux (IPCMS), UMR 7504 CNRS, Bat 70, 23, rue du Loess, 67034 Strasbourg Cedex, France

 $^3\mathrm{LEM},$ ONERA-CNRS (UMR104), 29 av. De la Division Leclerc, BP 72, 93322 Chatillon Cedex, France

High resolution near edge X-ray absorption fine structure (NEXAFS) spectroscopy have been used to investigate the nitrogen doping of multi wall and single wall carbon nanotubes. NEXAFS spectroscopy at the nitrogen K-edge reveals three different chemical bonding of the nitrogen similar for both single and multiwall nanotubes. In particular pyridine-like structure is clearly exhibited. The relative concentration of the different chemical environments of the nitrogen is clearly different for single and multi wall nanotubes. High resolution NEXAFS experiments show that the main nitrogen concentration observed for multi wall carbon nanotubes originates from a high amount of molecular N2 encapsulated into the tubes and adsorbed at the surface of the internal tube.

10 Investigation of Sodium Dodecyl Benzene Sulphonate Assisted Dispersion and Debundling of Single Wall Carbon Nanotubes.

PRIYA BASKAR RAO

FOCAS, DUBLIN INSTITUTE OF TECHNOLOGY, DUBLIN

The dispersion limit of HiPco Single Wall Carbon Nanotubes in 1 percentage by weight Sodium Dodecyl Benzene Sulphonate assisted dispersions in water is reported. The starting concentration of the tubes in water surfactant solution was 5 mg per ml which was diluted sequentially by a factor of 2 down to 0.0012 mg per ml. Sonication and centrifugation were performed to obtain a homogenous dispersion of HiPco SWCNTs in water surfactant solution. Concentration dependent absorption and Raman spectroscopic studies were used to analyse the SWCNTs behaviour in water based solution, and AFM was employed to examine the aggregation state of the nanotubes over the concentration range. Both spectroscopic techniques demonstrate a clear concentration below which the nanotube bundles become significantly dispersed in the solution. The concentration limit at which debundling starts was

found to be 0.07 plus or minus 0.03 mg per ml. The dispersion behaviour and optical parameters determined are compared with those established for other solvent media

11

Quantum Conductance in Carbon Nanotube Networks

Mark Baxendale¹ Zahra Alemipour¹

¹Queen Mary, University of London, London

The electrical conductance of single- and double-wall carbon nanotube systems was measured by a mechanically controllable break-junction technique using free-standing nanotubes not subject to any chemical modification. For metallic single-wall carbon nanotubes two channels with transmission coefficient 0.88 - 1 contribute to ballistic electronic transport at room temperature. In double-wall carbon nanotubes, one metallic channel contributes to ballistic electronic transport and an additional field- and temperature-dependent two-channel contribution was observed. Multi-wall carbon nanotubes were found to have a broad range of conductance behaviour dependent on the number of walls and crystalline quality.

12

Electrostatic Modeling of Carbon Nanotubes in Asymmetric Electric Fields Sabine Blatt¹ Aravind Vijayaraghavan¹ Ralph Krupke¹

¹Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Recently, high density arrays of single walled carbon nanotube (SWNT) devices have been produced by the deposition of individual nanotubes between a biased electrode and an electrically floating counter electrode. [1] After depositing a nanotube, this constitutes a 3-terminal device with the biased electrode acting as source, the floating electrode forming the drain and the underlying silicon substrate the gate. Application of a gate-source potential then leads to an asymmetric potential profile along the nanotube which affects the charge distribution on the nanotube.

We use finite element simulation to model the potential profile and charge distribution for a semiconducting nanotube in such a device. [2] Since we are interested in the equilibrium situation where the net currents are zero, it is sufficient to solve self-consistently the Poisson equation taking induced charges on the nanotube into account.

We compare 2d, 3d cylindrical and 3d cartesian geometries to explore the influence of the floating electrode. The results for planar devices with asymmetric bias are compared to experimental observation of charge distribution by voltage contrast scanning electron microsopy.[3]

1 A. Vijayaraghavan et al., Nano Letters 7, 1556-1560, 2007

- 2 D. L. John et al., IEEE Trans. Nanotechnol. 2, 175-180, 2003
- 3 A. Vijayaraghavan et al., Visualizing Electronic Properties of Carbon Nanotube Devices by Voltage Contrast Scanning Electron Microscopy, IWEPNM 2008

Single-walled Carbon nanotubes as anticancer drug delivery system

Ewa Borowiak-Palen¹ Carla Tripisciano¹

¹Institute of Chemical and Environment Engineering, Szczecin University of Technology, Szczecin

Conventional administration of chemiotherapeutic agents is frequently impaired by their lack of selectivity and accidental damage inflicted to healthy tissues. Since Carbon Nanotubes possess the unique feature of being able to enter a living cell without causing its death, they can be used to deliver small organic drug molecules into the deseased cells not damaging the healthy ones. Thus therapeutic and diagnostic agents can functionalize the structure of carbon nanotubes. Here, the functionalization of Single-Walled CNTs with Cisplatin (Cis-Diamminedichloroplatinum (CDDP) - a platinum based chemotherapy drug used to treat various types of cancers) is presented. The purity of SWCNTs sample was estimated with thermogravimetric (TGA)study and the remaining amount of the catalysts were analysed with atomic absorption spectroscopy (AAS) The morphology characterization was carried with X-ray diffraction (XRD) and high resolution transmission electron microscopy (HR-TEM). The sample chemical composition analysis was performed with energy dispersive X-Ray spectroscopy (EDX). Raman Spectroscopy was exploited to observe whether Cisplatin was placed on SWCNTs external surface or inside the tubes. Additionally, the CDDP release from the samples in physiological solution was studied using inductively coupled plasma(ICP) analysis.

14

INFLUENCE OF NITROGEN DOPING ON FIELD ELECTRON EMISSION AND LITHIUM INTERCALATION OF CARBON NANOTUBES

<u>Lyubov G Bulusheva</u>¹ Alexander V Okotrub¹ Alexander G Kurenya¹ Olga V Sedelnikova¹ Ian Kinloch² Huaihe Song³

Arrays of multiwall carbon nanotubes (CNT) and nitrogen-doped carbon (CNx) nanotubes have been synthesized by aerosol CVD method with injection of ferrocene solution in toluene, acetonitrile and in a mixture of toluene and acetonitrile. X-ray photoelectron spectroscopy estimated the CNx nanotubes produced from

¹Nikolaev Institute of Inorganic Chemistry, Novosibirsk

²School of Materials, The University of Manchester, UK

³Beijing University of Chemical Technology, P.R. China

pure acetonitrile contain 6% of nitrogen. Raman spectroscopy showed increase of intensity ratio of D and G modes with enhancement of nitrogen concentration in CNx nanotubes. The measurements of filed emission characteristics of the samples produced demonstrated lowering of the applied voltage threshold with nitrogen doping of CNT. Quantum-chemical calculations on carbon nanotubes incorporated three-coordinated nitrogen atoms and pyridinic-like nitrogen, performed within density functional theory (DFT), found the first kind of nitrogen atoms should provide improvement of field emission characteristics of CNx nanotubes. Theory predicts decrease of voltage threshold till nitrogen concentration in CNx nanotubes is lower than 4%. The measurements of charge-discharge characteristics on CNT and CNx nanotubes showed increase of lithium capacity for nitrogen-doped nanotubes. By the results of DFT calculations the lithium cation more readily interacts with pyridinic-like nitrogen. We found that lithium can penetrate inside of CNx nanotube through the atomic vacancy, which zigzag boundaries are presented by nitrogen atoms. The estimated barrier for intercalation of nitrogen-doped nanotube with lithium cation is 1.35 eV.

15 Nanotubes in macrophages: imaging and chemical analysis by micro X-ray fluorescence

<u>Julien Cambedouzou</u>¹ Cyrill Bussy¹ Sophie Lanone² Emilie Leccia¹ Mathieu Pinault³ Martine Mayne l Hermite³ Marine Cotte⁴ Jean Doucet¹ Jorge Boczkowski² Pascale Launois¹

¹Laboratoire de Physique des Solides, Université Paris Sud XI, Orsay, France

²INSERM, Unit 700, F-75018 Paris, France

³LFP, URA CEA-CNRS 2453, CEA Saclay, F-91191 Gif/Yvette, France

⁴ESRF, F-38043 Grenoble, France

A growing concern about the potential human health impact associated with carbon nanotubes (CNT) in occupational environment emerges. One key-issue in understanding CNT biological effects is to characterize their interactions with cells. A prerequisite is the localization of CNTs in cells [1]. A second point is to have information about cell modifications after contact with CNTs. Both points can be addressed using synchrotron-based micro X-ray fluorescence (μ XRF), used here for the first time to study CNT-cell interactions [2]. Experiments have been performed for exposition of murine macrophage to either SWCNTs or MWCNTs, the choice of macrophage cells being dictated by their crucial role in inflammation and respiratory responses to exogenous agents.

Analysis of the fluorescence signal of iron catalyst particles attached to the nanotubes gives information about their cell localization. A dose-response effect is measured for the cellular iron signal in CNT-exposed cells. In some of the exposed cells, an additional calcium signal is observed, which also seems to follow a dose-response pattern. This finding could be of strong importance in the perspective of

understanding the toxicological effects of CNTs, since excess of calcium could be linked to functional disorder like cytotoxicity, oxidative stress and inflammation [3]. Accordingly, first pharmacological assays with calcium chelators and inhibitors show a role of calcium on cytotoxity and cell inflammatory response after exposure to CNT.

- 1 A. E. Porter, M. Gass, et al., Nature Nanotechnology 2007, 2, 713
- 2 C. Bussy, J. Cambedouzou, et al., submitted
- 3 D.M. Brown, L. Hutchison, et al., Am. J. Physiol. Lung Cell. Mol. Physiol. 2007, 292, L1444

16

A two-step mechanism for the oxidation of vacancies in graphene

<u>Johan M. Carlsson</u>¹ Felix Hanke¹ Matthias Scheffler¹

¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Complete oxidation of graphitic carbon materials leads to combustion and the formation of CO₂, but it has been suggested that partial oxidation of vacancies on the basal plane can yield catalytically interesting materials. The characterization of such oxidized graphite in temperature-programmed desorption (TPD) experiments detected a surprising amount of CO and significantly less CO₂ [1]. This work aims to clarify the oxidation mechanisms and surface structures under different experimental conditions.

We use density functional calculations with PBE exchange-correlation to obtain the structural and energetic properties of oxidized graphene vacancies. To understand the TPD spectra, reaction barriers and rates for CO and CO₂ desorption are calculated from transition state theory and the nudged elastic band method. An *ab-initio* thermodynamics analysis shows a significant partial pressure-dependence of the oxygen content in vacancies. This indicates a two step mechanism for the initial oxidation, by which strongly bound CO-releasing C-O-C and C=O groups saturate the vacancies under the ultra-high vacuum conditions of TPD experiments. Atmospheric partial pressures lead to additional oxygen adsorption into extended groups such as C-O-C=O and O=C-O-C=O, which in return can desorb as CO₂, with a lower desorption barrier than the CO-desorption from the C-O-C and C=O groups.

1 B. Marchon et al., Carbon **26**, 507 (1988).

Seeing and counting graphene layers with Rayleigh scattering

A. Hartschuh¹ H. Qian¹ H. Harutyunyan¹ T. Gokus¹ E. Lidorikis² K. S. Novoselov³ C. Casiraghi⁴ A. C. Ferrari⁴

¹Chemistry and Biochemistry Department, Munich University, Munich, Germany ²Department of Materials Science and Engineering, University of Ioannina, Ioannina, Greece

³Department of Physics and Astronomy, Manchester University, Manchester, UK
⁴Engineering Department, Cambridge University, Cambridge, UK

Developing tools for quick, non-destructive identification of graphene layers is key to enable graphene technology. Raman scattering has emerged as an ideal, nondestructive technique for the identification of graphene and its doping [1, 2]. However, the Raman scattered photons are a minority compared to those elastically scattered. Elastic scattering (Rayleigh scattering) can provide a much quicker means of identification of single and multi-layer samples. Here we report an extensive investigation of graphene by monochromatic and white-light Rayleigh scattering and the theoretical understanding of the experimental data [3]. Samples consisting of increasing number of layers are identified by a combination of AFM and Raman Spectroscopy. Confocal Rayleigh maps are obtained by raster scanning the sample with a piezoelectric stage. The scattered light depends on the dielectric function of the samples and their geometry. In particular we show that i) for a given interface layer, the graphene contrast can be tailored by adjusting its thickness; ii) for a given interface thickness, the contrast can be maximized by changing interface material, such as SiN instead of SiO2; iii) for a given interface material or thickness, the contrast can be maximized by changing the wavelength of the incident light; iv) In all cases, the contrast strongly depends on the graphite thickness and the intensity varies with the number of layers. Using this technique, large graphene layers can be mapped and identified in a few minutes. Furthermore, graphene imaging can also be efficiently accomplished by using standard microscopy and a set of light filters.

- 1 A. C. Ferrari et al., Phys. Rev. Lett.97, 187401 (2006).
- 2 S. Pisana et al., Nature Materials 6, 198 (2007).
- 3 C. Casiraghi et al. Nano Letters 7, 2711 (2007).

18

Electronic properties of functionalised graphene nano-ribbons

Felipe Cervantes-Sodi¹ Gabor Csanyi¹ Stefano Piscanec¹ Andrea C. Ferrari¹ Engineering Department, University of Cambridge, Cambridge

Graphene nanoribbons (GNRs) can be regarded as the counterpart of carbon nanotubes in graphene-based nanoelectronics [1]. The electronic properties of GNRs

are determined by the geometry of the edges [2] (zigzag, armchair or a combination of the two), and can be perturbed and modified by chemical disorder [3].

Here we present a detailed investigation, of the electronic properties of GNRs performed by density functional theory calculations. In particular, we focus on the effects of edge functionalization (single-sided and double-sided), chemisorption, adsorption and atomic substitutions [3].

We find that single edge functionalization of zigzag ribbons with NO_2 , NH_2 , COOH and OH radicals does not introduce impurity levels in the band gap, but breaks the spin degeneracy. This can result in the onset of either a half-semiconducting state -with two spin channels having a different band gap- or a spin-polarized half-semiconducting state -where the spin in the valence and conduction bands are oppositely polarized [3]. On the contrary, we find that oxygen edge-functionalization and oxygen edge-substitution in zigzag ribbons induces a semiconductor-metal transition. A semiconductor-metal transition also happens with nitrogen bulk substitution in a NH_2 edge functionalized zigzag ribbon.

For armchair ribbons, we find that edge functionalization and edge atomic substitution modify the size of the band gap only by a few percent. On the contrary, nitrogen and boron bulk substitution can significantly shift the Fermi energy, inducing a semiconductor-metal transition.

Finally, we also report the effect of H_2O and O_2 adsorbed molecules as well as H and OH chemisorbed radicals on the ribbons electronic structure.

- 1 A. K. Geim, K. S. Novoselov, Nature Materials, 6, 183 (2007).
- 2 Y.-W. Son, M. L. Cohen, S. G. Louie; Phys. Rev. Lett., 97, 216803 (2006).
- 3 F. Cervantes-Sodi, G. Csanyi, S. Piscanec, A. C. Ferrari; arXiv: 0711.2340 (2007).

19

Solubilisation of Single-Walled Carbon Nanotubes in organic solvents

H. J. Byrne¹ S. Debnath¹ E. Gregan¹ Qiaohuan Cheng¹

¹Dublin Institute of technology, Dublin Institute of technology, Dublin

Significant effort has been devoted to looking for suitable media in which as produced or modified SWNTs can be dissolved to a useful concentration. Organic solvents which can directly interact with the side wall of SWNTs have attracted significant interest in the recent years. Amongst previous studies into organic solvents, amide solvents have been systematically studied [1]. However the solubility of SWNTs is not as high as that reported for some aromatic solvents such as monochlorobenzene and 1,2dichlorobenzene. Motivated by this observation, a systematic study of the effect of aromatic solvents on the dispersion of HiPco SWNTs has been conducted. Chlorine substituted benzene solvents such as monochlorobenzene,

1,2dichlorobenzene, 1,3dichlorobenzene and 1,2,4trichlorobenzene are investigated first. UV/vis/NIR spectroscopy equipped with an integrating sphere is employed to investigate the debundling concentration. For each solvent, a concentration dependent study of absorbance and scattering demonstrates a clear transition between aggregates and dispersed tubes. Raman spectroscopy and Atomic Force Microscope (AFM) are used to demonstrate the spectral differences above and below debundling point and thus give a confirmation of the debundling. A critical examination of the efficacy of the solvents in dispersing and solubilising the nanotubes is presented.

1 Landi, B.J. et al, Effects of alkyl amide solvents on the dispersion of single-wall carbon nanotubes. J. Phys. Chem. B, 108, 17089 (2004)

20

Environmental Effects of the Photoluminescence Spectra from Suspended Single-walled Carbon Nanotubes

 $\underline{\rm Shohei~Chiashi}^1$ Tateki Hanashima 1 Kotaro Nagatsu 1 Kyo Kanahori 1 Yoshikazu Homma 1

¹Tokyo University of Science, Tokyo

We measured the photoluminescence (PL) spectra from the suspended single-walled carbon nanotubes (SWNTs) between the pair of the quartz pillars, and investigated their environmental effects. In ethanol gas atmosphere, the PL spectra were dependent on the gas pressure and showed a rapid energy shift at a gas pressure (transition pressure). The transition pressure was dependent on temperature and the tube diameter, and the PL peak did not depend on the pressure below the transition pressure. The gas pressure dependence was explained by adsorption and desorption phenomena of ethanol molecules on SWNT surface, because the adsorbed ethanol molecules changed the dielectric constant surrounding the SWNT. On the other hand, when the SWNT surface was deposited with small metal particles, a small peak appeared on the long-wavelength side of the main peak. The deposited material would slightly deform the SWNT structure and the emission from the lower energy state was enhanced.

21

Carbon nanotube nanomechanical mass sensors

Hsin-Ying Chiu¹ Peter Hung¹ Henk Postma² Marc Bockrath¹

Single-walled carbon nanotubes are arguably the lightest and smallest wires in the world, and have recently been shown to act as nanomechanical resonators [1]. As a result, single-wall carbon nanotubes are excellent candidates for highly sensitive mass sensing [2].

¹California Institute of Technology, Pasadena

²California State University, Northridge

We observed the down shift of the resonant frequency of a suspended double-clamped carbon nanotube resonator at cryogenic temperatures upon helium mass loading. Using a straightforward estimate of the nanotube mass, the observed frequency shift corresponds to the mass of 1000 helium atoms, which is the zeptogram range. This is considerably smaller than found previously with nanotube resonators, and comparable to that found using nanowire resonators [3]. Our noise floor is currently Xenon atom per root Hz, which may enable single-atom detection in future experiments. Experiments to detect individual atoms or molecules are ongoing; our latest results will be presented.

We also observe discrete features of resonant frequencies and non-monotonic dependence of frequency on gate voltage. We attribute this to Coulomb blockade at cryogenic temperatures.

- 1 Vera Sazonova, et al., Nature 431, 284 (2004).
- 2 H. B. Peng, et al. Phys. Rev. Lett. 97, 087203 (2006)
- 3 Y. T. Yang, et al. Nano Lett. 6, 583 (2006).

22

Fullerene transformations in peapods under extreme conditions

<u>Matthieu Chorro</u>¹ J. Cambedouzou¹ A. Iwasiewicz-Wabnig² L. Noe³ S. Rols⁴ M. Monthioux³ B. Sundqvist² P. Launois¹

 $^1\mathrm{Laboratoire}$ de Physique des Solides, UMR CNRS 8502, Universite Paris Sud, 91405 Orsay, France

²Department of Physics, Umea University, 90187 Umea, Sweden

³Centre d Elaboration des Materiaux et d Etudes Structurales, UPR CNRS 8011, 31062 Toulouse, France

Nanostructures obtained by the insertion of molecules in the hollow cavity of single-walled carbon nanotubes (SWNT) give to the scientific community the opportunity of studying original confined quasi-1D phases [1]. When inserted molecules are fullerenes, resulting nanostructures are called peapods, the structure reminding pods (nanotubes) full of peas (fullerenes). Different kinds of peapods are synthesized according to the nature of the molecule inserted, for instance the spherical C60 molecule or the egg-shaped C70 molecule. In this study, we focus on the fate of the fullerene confined inside SWNT when they are submitted to high pressure and/or high temperature (HPHT) conditions. In a first part, we show ex situ X-ray diffraction results from peapods having been exposed to HPHT conditions. Same HPHT treatments were applied to both C60 peapods and C70 peapods. We observed that confined C60 polymerize inside the nanotubes for the same temperature/pressure range than bulk C60. However, we did not observe any polymerization of C70 molecules, even for HPHT conditions leading to polymerization in the bulk C70 phase.

⁴Institut Laue Langevin, 38042 Grenoble, France

The different structural behaviours observed for C60 and C70 peapods after extreme conditions is explained in terms of geometrical arguments. Our results testify for the strong influence of the confinement inside the nanotube on the orientational ordering and on the chemistry of the C70 molecules [2]. In a second part, we will focus on the high temperature activated transformation from peapods to double-walled carbon nanotubes (DWNT). The fine X-ray diffraction analysis of DWNT resulting of the coalescence of both C60 and C70 chains shows that the structure of the DWNT is not influenced by the type of starting fullerene. This result, together with the determination of the structural parameters of the DWNT, allows us to discuss the possible scenario for the growth of the inner tube from fullerenes.

- 1 A.N. Khlobystov, D.A. Britz, et al., Acc. Chem. Res. 2005, 38, 901
- 2 M. Chorro, J. Cambedouzou, et al., Europhys. Lett. 2007 79, 56003

23

Electron spin resonance study of single walled nanotubes filled with La@C₈₂ Jamie Warner¹ Andrew Briggs¹ <u>Luka D Ciric</u>² Andrzej Sienkiewicz² Katarzyna Pierzchala² Balint Nafradi² Arnaud Margez² Alexandar Duncan² Laszlo Forró²

¹Department of Materials, University of Oxford, Oxford, UK

We report ESR studies on La@C₈₂ and La@C₈₂ filled peapods. The latter material was investigated for applications in quantum information processing. The ESR spectra were measured at X- and Q-bands in the temperature range from 4K to 295K. The ESR spectrum of La@C₈₂ in CS₂ shows hyperfine splitting of 8 lines, having the linewidth of 0.15G at room temperature. We also studied the photo-catalytic properties of La@C₈₂ in CS₂ and we found that under illumination with white light La@C₈₂ does not generate singlet oxygen via type II energy transfer. For preparing peapods from spin-active La@C₈₂ fullerenes the starting material was mixed with C₆₀ in 1-10% proportions to avoid spin-spin interaction broadening. ESR studies on peapods were performed for 1, 5, 10 and 100% of La@C₈₂ in C₆₀. Filling of SWCNTs was also tracked by TEM and the results were related to parallel ESR observations. Acknowledgment: This work is performed in the frame of the European network IMPRESS. The endohedral fullenes from the Shinohara-group is gratefully acknowledged.

24

Time-Correlated Single Photon Counting of Structurally Sorted Single-Wall Carbon Nanotube Suspensions

 $\underline{\text{Michael Clemens}}^1$ Jared Crochet¹ Tobias Hertel¹

²Institute of Complex Matter - Labaratory for novel electronic materials, EPFL Ecole Polytechnique Federal de Lausanne, Lausanne

¹Department of Physics and Astronomy, Vanderbilt University, Nashville, TN, USA

We present preliminary results from a time-correlated single photon counting study of structurally sorted single-wall carbon nanotube suspensions. Photoluminescence decay times of different types of carbon nanotube suspensions are determined with 5 ps time-resolution. For structural sorting we use density gradient ultracentrifugation. This technique allows to not only isolate individual SWNT-micelles from SWNT aggregate-micelles and SWNT-crystallites (or bundles) which are present in the supernatant of typical nanotube suspensions but it also allows to isolate SWNT aggregates with different buoyancy. We use samples of nanotube aggregates with specific buoyancy to study the gradual decrease of PL quantum yields and the associate changes in PL decay times as a function of increasing SWNT crystallite size. The results clearly illustrate why early measurements suggested that PL quantum yields on the order of 10^{-3} or even 10^{-4} are nearly two orders of magnitude smaller than yields in excess of 10^{-2} obtained for todays best structurally sorted samples.

25

Electronic properties of catalyst-free SWNT probed by resonant and non-resonant microwave absorption

B. Corzilius¹ K.-P. Dinse¹ K. Hata²

¹Physikalische Chemie III, Technische Universität Darmstadt, Petersenstr. 20, D-64291 Darmstadt, Germany

²AIST, Tsukuba Central 5, Tsukuba 305-8565, Japan

Using electron paramagnetic resonance (EPR) it was possible to identify two different temperature regimes of the electronic properties of bulk samples of single wall carbon nanotubes [1-3] synthesized by 'super-growth CVD method [4]: at high temperatures the spectrum shows clear evidence for the presence of itinerant spins with a freezing temperature of about 100 K; below this temperature the spectrum is dominated by localized spins not detectable at higher temperatures. At very low temperatures (T < 12 K) the samples show strong non-resonant and non-linear mw absorption. This behaviour is interpreted as indicative for the formation of a superconducting phase of a part of the sample. In addition, a part of the sample shows a magnetic ordering transition at a somewhat higher temperature, which can be suppressed by the application of a small magnetic field. We also found evidence for the existence of a metastable state at low temperatures, which shows a distinct creeping behaviour in the time-scale of several hours. The occurrence of this metastable phase can be controlled by sample treatment with molecular oxygen at ambient conditions and heating of sample under vacuum.

- B. Corzilius, K.-P. Dinse, J. van Slageren, K. Hata, Phys. Rev. B 75, 235416 (2007).
- 2 B. Corzilius, K.-P. Dinse, K. Hata, Phys. Chem. Chem. Phys. 9, 6063 (2007).

- 3 B. Corzilius, S. Agarwal, K.-P. Dinse, K. Hata, phys. stat. sol. (b) 244, 3890 (2007)
- 4 K. Hata, D. N. Futaba, K. Mizuno, T. Namai, M. Yumura, S. Iijima, Science 306, 1362 (2004).

Internalisation of Carbon Nanotubes into Human Embryonic Stem Cells ${\rm Alan\ Dalton}$

Department of Physics, University of Surrey, Guildford

Silencing Efficiency, Toxicity and Potential Applications Carbon nanotubes (CNTs) are showing increasing versatility for the cellular internalization and delivery of biological agents including proteins, antibodies, polynucleotides and more. Combinations of these agents may lead to advanced drug delivery transporters for a variety of in vitro and in vivo biological applications. While work advances for CNTs, human embryonic stem cells (hESCs) hold much potential for drug screening applications, regenerative therapy, and new generations of medicine. Fundamental understanding of hESCs functioning and development focus on the roles active genes assert over the inner mechanisms of the cells, and silencing of these genes shed new understanding on the role they play. While current gene silencing and transfection methods often damage the cell populations viability and growth or have low silencing efficiencies, CNT transporter schemes have been shown to surpass commercially available transfection agents with neglible detrimental effects to the cells. Here in we report the cellular internalization, silencing efficiency, and toxicity effects of CNTs for hESCs.

27

An experimental study of the interaction between single walled carbon nanotubes and polycyclic aromatic hydrocarbons.

Sourabhi Debnath¹ Q. Cheng¹ T. G. Hedderman¹ H.J. Byrne¹ Dublin Institute of Tecnology, Dublin Institute of Tecnology, Dublin

Single-walled carbon nanotubes (SWNTs) are proposed to be the most promising of all nanomaterials, with unique electronic and mechanical properties which lend themselves to a variety of applications. In all cases the quality of the SWNTs material is important, and for some applications it is paramount. There are several production processes of SWNTs. Despite sustained efforts, all currently known SWNTs synthetic techniques generate significant quantities of impurities. They also grow in bundles or ropes and are largely insoluble in common organic solvents. SWNTs can have a range of structures and their electronic properties depends on their structure and as well as their diameter. Currently there is no production process that can produce only one particular type of SWNTs. Due to these reasons

carbon nanotubes have been slow to reach real potential applications. To speed up the potential applications of SWNTs it has now become mandatory to purify, increase the solubility, disperse and separate SWNTs according to their electronic properties. It has been found that organic solvents in the presence of organic dyes such as polycyclic aromatic hydrocarbons (PAHs) can easily interact with SWNTs and the solubility of SWNTs are increased in the solvent [1]. This process is also used to purify and disperse SWNTs from their bundles. In this work dyes of two oligomer series, the acene series and phenyl series, are used to study the interaction between SWNTs and organic dyes.

The interactions and debundling of SWNTs are investigated through spectroscopic methods such as fluorescence. The fluorescence concentration dependence studies define the concentration range where aggregated dyes and isolated dies exist. A fluorescence model based on the fraction of free hydrocarbons is used to indicate the concentration range where isolated and bundled SWNTs and organic dyes are interacting [2]. By using this model the binding energy between SWNTs and organic dyes is also obtained.

- 1 Hedderman, T.G., S.M. Keogh, G. Chambers, and H.J. Byrne, In-depth study into the interaction of single walled carbon nanotubes with anthracene and p-terphenyl. Journal of Physical Chemistry B, 2006. 110(9): p. 3895-3901.
- 2 Coleman, J.N., A. Fleming, S. Maier, S. OFlaherty, A.I. Minett, M.S. Ferreira, S. Hutzler, and W.J. Blau, Binding kinetics and SWNT bundle dissociation in low concentration polymer-nanotube dispersions. Journal of Physical Chemistry B, 2004. 108(11): p. 3446-3450.

28

Modification of electrical properties of SWNT bucky paper by heavy ion irradiation

<u>Urszula Dettlaff-Weglikowska</u> Viera Skakalova Kai Arstila Arkady Krasheninnikov Siegmar Roth

Samples of SWNT mats, called bucky paper, have been irradiated with a $^{12}\mathrm{C}^{+4}$ ion beam in order to improve their mechanical stability. Investigations by Raman spectroscopy show that the irradiation creates sp3 defects. The intensity of the D mode line inreases continuously with increasing the irradiation dose. The ion beam irradiation changes also electrical properties of the backy paper. The conductivity measured at room temperature decreases with the irradiation time. The temperature dependence of conductivity indicates changes in the conduction mechanism. Whereas the pristine sample exhibits mixed metallic-nonmetallic character according to fluctuation assisted tunneling, the irradiated samples change to semiconducting behavior described by variable range hoping.

¹Max-Planck-Institute for Solid State Research, Stuttgart, Germany

²University of Helsinki, Helsinki, Finnland

Synthesis of vertically aligned single-walled carbon nanotubes and their anomalous Raman spectra

 $\underline{\text{Erik Einarsson}}^1$ Zhengyi Zhang 1 Rong Xiang 1 Kazuaki Ogura 1 Jun Okawa 1 Shigeo Maruvama 1

¹Dept. of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656 Japan

We review our recent studies on the synthesis of vertically aligned single-walled carbon nanotube (VA-SWNT) films by chemical vapor deposition (CVD) of alcohol [1]. In particular, we look at how the ethanol pressure affects the growth process in real-time using an *in situ* optical absorbance measurement [2]. We find there is an optimum ethanol pressure that increases with CVD temperature, below which the growth is governed by a first-order reaction. The growth rate of the film is also found to be sensitive to changes in the growth environment, and can change on short time scales. We also report preliminary results from polarized Raman spectroscopic studies that show anomalous anisotropic behavior in the radial breathing mode. A possible connection between this anisotropy and the small-bundle structure of the VA-SWNT films [3] is discussed.

- 1 Y. Murakami, S. Chiashi, Y. Miyauchi, M. Hu, M. Ogura, T. Okubo, S. Maruyama, *Chem. Phys. Lett.* **385** (2004) 298.
- 2 S. Maruyama, E. Einarsson, Y. Murakami, T. Edamura, *Chem. Phys. Lett.* **403** (2005) 320.
- 3 E. Einarsson, H. Shiozawa, C. Kramberger, M.H. Rümmeli, A. Grüneis, T. Pichler, S. Maruyama, *J. Phys. Chem. C* 111 (2007) 17861.

30

Boson-controlled quantum transport in electronically low-dimensional materials

Holger Fehske¹ Andreas Alvermann¹ David M. Edwards²

The interplay of collective dynamics and damping in the presence of correlations and bosonic fluctuations is studied within the framework of a newly proposed model, which captures the principal transport mechanisms that apply to a variety of physical systems. The close connections to the transport of lattice and spin polarons, or the dynamics of a particle coupled to a bath are established. The model is analysed in the one-particle sector by exactly calculating the optical conductivity, Drude weight, inverse photoemission spectra, quasiparticle mass and band dispersion, as well as particle-boson correlation functions, for finite and infinite one-dimensional

¹Institut für Physik, Ernst Moritz Arndt Universität, Greifswald, Germany

²Department of Mathematics, Imperial College, London, United Kingdom

systems. For the half-filled band case a metal-insulator quantum phase transition is proved to exist.

31

Electron-Electron Interaction, Electron-Phonon Coupling Renormalisation and the Raman spectrum of Graphene

A. C. Ferrari¹ S. Piscanec¹ D. M. Basko²

¹Engineering Department, University of Cambridge, Cambridge

Recent years have seen a steady advance in the understanding of the Raman spectra of carbon-materials. This includes the double resonance mechanism for the activation of the D and D' peaks around \mathbf{K} and Γ [1], and the presence of Kohn anomalies for phonons at \mathbf{K} and Γ induced by their large electron-phonon coupling (EPC) [2]. The latter explain, e.g., the G Peak doping dependence and the different behaviour of the G^+ and G^- peaks, with wider implications for electron and phonon transport [2,4].

Still, some basic facts remain unexplained. First, the intensity of the second order 2D peak in graphene is far higher than that of the 2D⁴, and strongly depends on doping [5]. Second, since the EPC cannot contribute to its broadening [4], the 2D peak should be extremely sharp compared to the G peak[4], in contrast with experiments. Third, the sum of the EPCs at \mathbf{K} and Γ is too small to account for the kinks observed in the ARPES spectra of graphene [6]. Since the calculated G peak EPC was experimentally validated [2-4], current DFT calculations may thus underestimate the EPC at $\mathbf{K}[2]$.

Here we show that all these results can be explained by taking into account Coulomb interactions when calculating the EPC. The key observations are that: (i) in fully resonant two-phonon Raman processes the generated electron-hole pairs can scatter not just with phonons, but also with electrons and holes [8], and this cannot be neglected, as done so far [2,4]; (ii) Coulomb interactions enhance the EPC of the D peak, but not that of the G peak [7]. We explain the experimental width, intensity, doping and excitation dependence of the 2D peak and show how these can be used to determine its EPC [9]. Our measured and calculated EPC is now a factor of two higher than previously predicted by DFT [2, 9].

Furthermore, we show that Raman spectroscopy can be used as simple tool for measurement of electron-electron interactions and lifetimes [7,9], getting values consistent with direct ARPES measurements for electrons of similar energy [9]. While here we focus on graphene, significant implications are also expected for nanotubes.

- 1 C. Thomsen, S. Reich, Phys. Rev. Lett. 85, 5214 (2000).
- 2 S. Piscanec Phys. Rev. Lett. 93, 185503, (2004); Phys. Rev. B 75, 035427 (2007).
- 3 S. Pisana et al. Nature Materials 6, 198 (2007).

²SISSA, Trieste, Italy

- 4 M. Lazzeri et al. Phys. Rev. Lett 95, 236802 (1995).
- 5 C. Casiraghi et al. Appl. Phys. Lett. 91, 233108 (2007); A. Das et al. ar-Xiv:0709.1174v1.
- 6 Bostwick et al. Nature Physics 3 36, (2007).
- 7 D. M. Basko and I. L. Aleiner, arXiv:0709.1927v1 (2007).
- 8 D. M. Basko, Phys. Rev. B 76, 081405 (2007).
- 9 S.Piscanec, D.M. Basko, A. C. Ferrari, submitted (2008).

Indirect exchange coupling between localized magnetic in carbon nanotubes

Mauro Ferreira

School of Physics, Trinty College Dublin, Dublin

The exchange coupling between localized magnetic moments indirectly mediated by the conduction electrons of metallic hosts often plays a significant role in determining the magnetic order of low-dimensional structures. For low dimensional metallic structures, such as nanotubes, this interaction is predicted to decay rather slowly. Ab-initio calculations have nevertheless been unable to reproduce this prediction. To clarify this matter, we make use of a simple theoretical formalism that describes the coupling of magnetic atoms adsorbed to the walls of a nanotube. While confirming the predicted long range of the exchange interaction, our formalism also points to situations in which the coupling may display unexpectedly shorter ranges. We show that the interaction range depends rather sensitively on the location of the magnetic moments, which explains the difficulty in probing the long range character of the indirect exchange coupling from standard ab-initio calculations. Finally, we show that time-dependent excitations of the magnetic moments lead to a dynamic coupling whose range may be far superior.

33

Impedance Characterisation of Carbon Nanotube Thin Films

Nuria Ferrer-Anglada¹ J. Perez-Puigdemont¹ S. Roth²

Transparent conducting single wall carbon nanotube (SWNT) thin films are of great interest, due to many applications under development, as they present a high electrical conductivity and 80-90 % transparency as well as they are flexible. They

¹Dept. Applied Physics - CRNE, Universitat Politecnica de Catalunya, Barcelona ²Max-Planck-Institut fur Festkorperforschung, Heisenbergstrasse 1, Stuttgart, Germany

could be useful as transparent electrodes, flexible transistors or sensors [1-3]. It has been reported that either the conductance or I(V) characteristics depend strongly on the amount of SWNT deposited on the substrate, and on chemical treatment [4-5]. Some applications of SWNT thin films or networks on a substrate at different frequencies are envisaged, with medical use or other. In order to be able to construct reproducible devices with similar conductance G(f) and impedance Z(f), it is important to relate the electrical properties with the amount of SWNT present in the network. We analysed different networks containing different amounts of SWNT, using an Agilent Impedance analyzer up to 0,2 GHz. The amount of SWNT per cm2 present have been determined from TGA, and is correlated to the transparency determined by optical spectroscopy.

- 1 N. Ferrer-Anglada, M. Kaempgen, S. Roth et al., Diamond and Rel. Mat, 13, 256 (2004).
- 2 E. Artukovic, M. Kaempgen, D.S. Hecht, S. Roth, G. Gruner, NanoLetters, 5, 757 (2005).
- 3 Z. Wu, Z. Chen, X. Du, J.M. Logan, A.G. Rinzler et al., Science, 305, 1273 (2004).
- 4 B.B. Parekh, G. Fanchini, G. Eda, M. Chhowalla, Appl. Phys. Letters 90, 121913 (2007).
- 5 A.B. Kaiser, V. Skakalova, S. Roth, Physica E, (2007).

34

Optical and electrical simulation of molecular layer systems

 $\frac{\rm Konstantinos\ Fostiropoulos^1\ Wolfgang\ Tress^1\ Christian\ Breyer^1}{^1\rm Hahn-Meitner-Institut\ Berlin\ GmbH,\ Glienicker\ Str.\ 100,\ 14109\ Berlin}$

The goal of this work is to create an optoelectronic simulation tool for molecular layer systems like organic solar cells (OSC) using macroscopic material properties and fundamental physical processes in the bulk as well as at interfaces. Exemplary, metal-phthalocyanine/C60 OSC on indium-tin-oxide substrates are studied. The impact of exciton and charge transport in the bulk, exciton dissociation at the donor-acceptor interface as well as charge transfer at the organic-inorganic interfaces is investigated. A transfer matrix algorithm and an exciton diffusion model (optical) were applied to fit external quantum efficiency data using merely optical constants as experimentally determined input. Furthermore a drift diffusion model for charge carriers (electrical) is applied to simulate I-V curves in order to give hints for optimization of alternative cell concepts. Important parameters like exciton diffusion lengths, charge carrier mobilities, HOMO/LUMO levels etc. can be estimated.

In-situ Vis/NIR spectroelectrochemistry of single-walled carbon nanotubes enriched with the (6,5) tubes

 $\underline{\text{Otakar Frank}}^1$ Ladislav Kavan 1 Alexander A. Green 2 Mark C. Hersam 2 Lothar $\overline{\text{Dunsch}}^3$

¹J. Heyrovsky Institute of Physical Chemistry, v.v.i., Academy of Sciences of the Czech Republic, Dolejskova 3, CZ-182 23 Prague 8, Czech Republic

²Dept. of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208-3108, USA

 $^3{\rm Leibniz}$ Institute of Solid State and Materials Research, Helmholtzstr. 20, D - 01069 Dresden, Germany

An in-situ optical Vis/NIR spectroelectrochemistry study was performed on single-walled carbon nanotubes (CoMoCat) enriched with (6,5) tubes via density-gradient ultracentrifugation, as described in [1]. Thin semitransparent solid films were prepared from the solution of sorted nanotubes by vacuum filtration and purification with water. Despite some bundling of the nanotubes appears after this procedure, the peaks corresponding to optical transitions of tubes with distinct chiralities may be observed in the spectra. The effects of electrochemical redox doping on the electronic state of the nanotubes was investigated in a potential window between -2 and +2 V vs. Fc/Fc⁺. The bleaching of ΔE_{11}^S and ΔE_{22}^S optical transitions is traced for particular tubes, which allows a partial quantification of changes in electronic density of states (DOS) caused by filling with electrons or holes. The experimental values can be compared with data obtained by DFT calculations [2].

- 1 M.S. Arnold et al. Nature Nanotech. 2006, 1, 60.
- 2 J. Kurti et al. IWEPNM 2008.

36

Ultrafast relaxation in MoSI nanowires

 $\frac{\text{Christoph Gadermaier}^1 \text{ Primoz Kusar}^1 \text{ Damjan Vengust}^1 \text{ Dragan Mihailovic}^1}{^1\text{Department of Complex Matter, Jozef Stefan Institute, Ljubljana}}$

MoSI nanowires are a prototypical one-dimensional material, due to their particularly weak interaction with their neighbours. Any application in optics or electronics relies on functional properties of the active material in a non-equilibrium situation and its relaxation to equilibrium. We studied ultrafast electron relaxation in oriented MoSI nanowire thin films with femtosecond pump-probe spectroscopy. Resonant excitation leads to a depletion of the ground state absorption, superimposed on a structured photoinduced absorption spectrum. The temporal evolution of this spectrum reveals a complex relaxation behaviour which involves three distinct states. We found a cascade relaxation through these states, and determined their lifetimes, which are 0.5 ps, 5 ps, and longer than 1 ns, respectively. We discuss the

possible electronic nature of these states and the implications for fast optical and electronic applications.

37 Non-Markovian decoherence of localized nanotube excitons by acoustic phonons

Christophe Galland¹ Alexander Högele¹ Hakan Tureci¹ Ataç Imamoğlu¹

Institute of Quantum Electronics, ETH Hönggerberg, Wolfgang-Pauli-Strasse 16, CH-8093 Zürich, Switzerland

We demonstrate that electron-phonon interaction in quantum dots embedded in one-dimensional systems leads to pronounced, non-Markovian decoherence of optical transitions. The experiments we present focus on the lineshape of photoluminescence from low-temperature axially localized carbon nanotube excitons. The independent boson model that we use to model the phonon interactions reproduces with very high accuracy the broad and asymmetric emission lines and the weak reddetuned radial breathing mode replicas observed in the experiments. The intrinsic phonon-induced pure-dephasing of the zero-phonon line is two orders of magnitude larger than the lifetime broadening and is a hallmark of the reduced dimensionality of the phonon bath. The non-Markovian nature of this decoherence mechanism may have adverse consequences for applications of one-dimensional systems in quantum information processing.

38 Probing the doping in metallic and semiconducting nanotubes by Raman

Paola Gava¹ A.M. Saitta¹ N. Caudal¹ M. Lazzeri¹ F. Mauri¹ IMPMC, Pierre et Marie Curie, Paris

By means of ab-initio calculations we determine the dependence on the doping of the G^- and G^+ Raman peaks for both metallic and semiconducting carbon nano tubes. The essential ingredient for the correct description of the vibrational properties is the inclusion of dynamical effects beyond the standard adiabate Born-Oppenheimer approximation. The fully ab-initio calculations essentially confirms the results we previously obtained via a simplified model for metallic tubes [1]. An analogous behavior is now determined for semiconducting tubes. Our findings are in agreement with several independent measurements (see e.g. [2]). We find an important increase of the G^- peak in metallic tubes and of the G^+ in semiconducting ones as a function of electron and hole doping. This implies that Raman spectroscopy can be used as a measure of the doping in both metallic and semiconducting tubes.

- 1 N. Caudal et al., Phys. Rev. B **75**, 115423 (2007).
- 2 A. Das et al., Phys. Rev. Lett. 99, 136803 (2007).

OPTICAL ABSORPTION SPECTRA OF BN-NANOSTRUCTURES

 $\underline{\text{P.N. Gevko}}^1$ A. V. Okotrub 1 L.G.Bulusheva 1 I.V. Yushina 1 L. Bresson 2 A. Loiseau 2

¹Nikolaev Institute of Inorganic Chemistry SB RAS, av.Ak.Lavrentieva 3, Novosibirsk 630090, Russia

²Laboratorie d Etude des Microstructures ONERA, 29 Avenue de la Division Leclerc 92322 CHATILION Cedex, France

Samples of single-wall and multiwall BN-nanotubes, amorphous and hexagonal BN have been investigated by optical absorption spectroscopy, transmission electron microscopy and atomic-force microscopy. It was revealed that optical absorption spectrum of as-prepared single-wall BN-nanotubes has three absorption bands at 6.2 eV, 5.4 eV and 4.45 eV. The last band is represented by superposition of two bands with energies 4.37 and 4.49 eV. Investigation of this sample by transmission electron microscopy showed a presence of 60-70% of single-wall nanotubes. To reveal the origin of the recorded absorption bands the spectra of reference samples of multiwall BN nanotubes, hexagonal BN and amorphous BN have been measured. Only a single band located at 6 eV was detected for amorphous BN sample while the samples of multiwall nanotubes and hexagonal BN were found to be characterized by two bands at 6.2 eV and 5.4 eV. Thus, it is possible to assume, that absorption bands with energies 4.37 and 4.49 eV are characteristic of single-wall BN-nanotubes. Effect of hydration of BN nanotube surface on optical absorption has been investigated. The spectrum of the sample kept in the water vapors during 15 mines showed no absorption bands. To remove water molecules the sample was heated in vacuum at temperature 300C. We found that after annealing the spectrum of the sample still has no detectable bands. As atomic-force microscopy showed the presence in the sample of tubular structures with average diameter 0.25 mkm we suggest formation of strong hydrogen bonds between water molecules and BN-nanotubes that drastically changes their electronic structure.

40

Electron spin and charge in Carbon Nanotube Quantum Dots

Georg Goetz¹ G. Steele¹ W.E. Vos¹ L.P. Kouwenhoven¹

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

In the past few years, great progress has been made in confining electrons in Quantum Dots (QDs) in Carbon Nanotubes (CNTs). We expect that the spin of a single electron in CNTs shows interesting new properties and may serve as Quantum bit with a very long coherence time. This is, because of the special properties of carbon (weak spin orbit coupling, no nuclear spin). Our experiments aim at measureing the relaxation time of an confined electron spin and manipulate the electron spin in a controlled way. Here, we show that we can use a Single Electron Transistor to detect

the charge of a single electron in a CNT QD. This is an important step, opening the door to many interesting experiments with single electrons. Furthermore, we report on our ongoing efforts to measure the electron spin relaxation time in CNT QDs. As well, we show a new approach to define very clean but still tunable QDs in a CNT.

41

Tunable Coulomb Blockade in Nanostructured Graphene

 $\frac{\rm Johannes~G\"uttinger^1~Christoph~Stampfer^1~Francoise~Molitor^1~Davy~Graf^1~Thomas}{\rm Ihn^1~Klaus~Ensslin^1}$

We have measured the Coulomb blockade effect and Coulomb diamonds on an etched, tunable single-layer graphene single electron transistor (SET)[1]. The device consisting of a graphene island connected via two narrow graphene constrictions is fully tunable by three lateral graphene side gates. The functionality of lateral graphene gates has been investigated in detail and a transport gap is found to exist in the narrow graphene constrictions. On the nanostructured SET Coulomb blockade resonances are observed for suitably tuned in-plane gates. From Coulomb diamond measurements a charging energy of 3.5 meV is extracted. For increasing temperatures we detect an intricate interplay between the temperature dependence of the transmission of the nanostructured graphene barriers and that of the Coulomb blockade resonances.

1 C. Stampfer, J. Güttinger, F. Molitor, D. Graf, T. Ihn, and K. Ensslin, APL, in print, arXiv:0709.3799, (2007)

42

Growth of CNTs by the Laser Assisted CVD method

Miroslav Halušska¹ Yves Bellouard¹ Luuk van Laake¹ Andreas Dietzel¹ Micro and Nano Scale Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands

We report on the growth of carbon nanotubes (CNTs) with a Laser-Assisted Chemical Vapor Deposition (LA-CVD) method. The basic concept is to use a laser beam to create a hot spot on the substrate surface to promote locally CNTs growth. Our LA-CVD reactor contains two optical systems allowing an independent focusing and positioning of two laser beams with different wavelengths. A CO2 laser (wavelength of 10.6 micro m) and a laser diode (wavelength of 800 nm) are operated in a cw regime and have maximal power of 10 W and 35 W, respectively. Ethylene is used as a carbon source. Its flow rate, and dilution with Ar are computer controlled. In order to reduce metal oxides, H2 is added into the gas flow. In this work, we synthesized CNTs on flat substrates composed from Si/Al2O3/metal catalyst or

¹Laboratorium für Festkörperphysik, ETH Zürich, Zürich

Si/SiO2/metal catalyst layers. The metal catalyst is deposited by PVD in the form of a 1-2 nm thin layer of Fe or Co. Raman spectroscopy and SEM were used to characterize the growth products. SWCNTs or/and MWCNTs have been obtained as two and three dimensional nonaligned networks as well as vertically oriented CNTs forests.

43 Eludicating the Dynamics of Carbon Nanotube Film Growth by In Situ X-Ray Scattering

A. John Hart¹ Eric Verploegen² Eric R. Meshot¹ Sang-Woo Han¹ University of Michigan, Ann Arbor, MI
 Massachusetts Institute of Technology, Cambridge, MA

We investigate growth of vertically-aligned carbon nanotube (CNT) forests by in situ X-ray scattering, and thereby elucidate the dynamics of catalyst particle coarsening, forest self-organization, temperature- and reactant-driven CNT structure evolution, and growth termination. A custom-built atmospheric-pressure CVD reactor featuring a resistively-heated substrate platform is mounted directly in the synchrotron beamline, enabling real-time grazing incidence (GI-SAXS) and transmission (SAXS, WAXS) scattering studies. Simultaneous laser measurement of the forest height captures the growth kinetics, the heated platform enables rapid temperature changes (100 °C/s) during annealing and growth, and the reactant gas is independently pre-treated to create active carbon species. Starting with a catalyst thin-film of Fe/Al₂O₃ on Si, we observe rapid coarsening of Fe at temperatures as low as 550 °C. CNT diameter and growth rate are directly proportional to the substrate temperature, and tuning of annealing and growth conditions using SAXS-derived diameter measurements reveals that CNT forests with mean diameters ranging from 4-20 nm can be grown from the same starting catalyst film thickness. Rapid changes of substrate temperature initiate simultaneous growth of bi-modal CNT diameter distributions within forests. Growth self-terminates abruptly, accompanied by a sudden loss of alignment at the CNT-substrate interface; this appears to be a universal chemical and/or mechanical signature in our experiments. Our apparatus and investigation technique offer significant potential to further understand the limiting mechanisms of CNT forest growth, and for rapid tuning of process conditions to engineer application-oriented structural characteristics of nanotubes and nanowires.

44

Fluctuation enhanced gas sensing on functionalized carbon nanotube thin films

Radu Ionescu¹ Zoltan Gingl² Pulickel M. Ajayan³ Peter Heszler⁴ Zoltan Konya⁵ Akos Kukovecz⁵ <u>Henrik Haspel</u>⁵ Jani Maklin⁶ Krisztian Kordás⁶ Tero Mustonen⁶ Robert Vajtai⁷ Robert Mingesz²

- ¹Department of Electronics, Electrical and Automatic Engineering, Rovira i Virgili University, Tarragona, Spain
- ²Department of Experimental Physics, University of Szeged, Szeged, Hungary
- $^3\mathrm{Department}$ of Mechanical Engineering and Materials Science, Rice University, USA
- ⁴Department of Optics and Quantum Electronics, University of Szeged, Szeged, Hungary
- ⁵Dept. of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary
- ⁶Microelectronics and Materials Physics Laboratories, Department of Electrical and Information Engineering, University of Oulu, Finland
- ⁷Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, Troy, USA

Thin films of functionalized single-wall carbon nanotubes were deposited on silicon chips by drop-coating and inkjet printing. These sensors were subjected to 1-100 ppm NOx, CO, H2S and H2O vapor in synthetic air. We have found relatively small changes in the electrical resistance of the films exposed to different test gases, however chemical classification of these could still be achieved. To this end pattern recognition technique (principal component analysis) was applied on the acquired power spectral density of the stationary resistance fluctuations of the sensors. This phenomenon is called fluctuation enhanced sensing and it can be used to increase the amount of information gathered from a carbon nanotube sensor device.

45 Electronic structure of a graphene monolayer grown by chemical vapour deposition on Ni(111)

Alexander Grüneis¹ Denis Vyalikh² Thomas Pichler³ Serguei Molodtsov² IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

²Institut fuer Festkörperphysik, TU Dresden, Mommsenstrasse 13, D-01069 Dresden, Germany

³Dept. of Physics, Vienna University

We employ chemical vapour deposition of propylene for the growth of high quality graphene monolayers on Ni(111). Inspecting the dispersion of the pi electrons in the supported graphene layer by angle-resolved photoemission, we observe a "kink-like feature which indicates a strong hybridization between the pi and d states of graphene and nickel, respectively. Upon deposition and gradual intercalation of potassium atoms into the graphene/Ni(111) interface, the kink-like structure becomes less pronounced pointing at a potassium mediated attenuation of the interaction between the graphene and the substrate. This points towards a doping induced transition from a strong hybridization regime to a rigid band shift model. The experimental ARPES spectra of the graphene@potassium@Ni(111) system are in excellent agreement to tight binding calculations.

Integrated 3-Dimensional Microelectromechanical Devices from Processable Carbon Nanotube Wafers

 $\underline{\text{Yuhei Hayamizu}^1}$ Takeo Yamada 1 Kohei Mizuno 1 Robert C. Davis 2 Don N. Futaba 1 Motoo Yumura 1 Kenji Hata 2

¹National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

 $^2\mathrm{Department}$ of Physics and Astronomy, Brigham Young University, Provo, UT, USA

We describe the successful controlled self-assembly of carbon nanotubes into closely packed and highly aligned 3-dimensional (3D) films that we denote as CNT wafers. From CNT-wafers, we fabricated a wide range of complex 3D nanotube structures spanning from CNT islands on substrates, suspended sheets and beams linking single or multiple horizontal planes, and 3D cantilevers. These structures, each fabricated from thousands of nanotubes, are few microns in size and can be further integrated into functional 3D nanodevices. Every fabrication step is parallel and scalable, and thus massive nanodevices can be made simultaneously. Our approach opens up a new opportunity to fabricate rational nanodevices with unprecedented structural complexities and functionalities, and represents a giant step towards economical, scalable, and realistic nanodevice systems.

47

Improving Separation Techniques for Single-Walled Carbon Nanotubes: Towards Monodisperse Samples

<u>Frank Hennrich</u>¹ Sergei Lebedkin¹ Kentaro Sato² Riichiro Saito² Manfred M. Kappes¹

¹Institut fuer Nanotechnologie, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen

²Department of Physics, Tohoku University, Japan

Separation techniques for single walled carbon nanotubes (SWCNTs) have become an important research field within the last few years, mainly for the reason that the synthesis of carbon nanotubes does not allow to grow nanotubes with 100This contribution aims at giving an overview over separation techniques we are currently using for SWNTs. It will discuss (i) how one can achieve separation due to different electronic properties (metallic, semiconducting), length, diameter and chirality via size exclusion chromatography, dielectrophoresis, density gradient centrifugation and selective dispersing, (ii) how those separation methods work for different SWNT materials from different sources (HiPco, Laser ablation, CoMoCat) and (iii) which parameters (pre-treatments, sonication, different surfactants) influence the separation efficiency. In particular evidence will be presented that we have achieved the isolation of only one (n,m)-species. Our most important characterization

tool for SWNT suspensions is photoluminescence mapping. The obtained linewidth extracted for different (n,m)-species from emission spectra at room temperature is broader than the theoretically predicted linewidth. Linewidth broadening can occur due to (i) bundles (tube tube interaction), (ii) solvent/surfactant tube interaction (inhomogeneous broadening), (iii) impurities (defects), (iv) finite length effects and (v) exciton phonon coupling. We have found evidence that for bundle-free SWNTs samples which contain defect-free, long tubes exciton phonon coupling is the major contribution to the linewidth broadening.

48

Ultrafast exciton dynamics in carbon nanotubes

<u>Tobias Hertel</u>¹ Katharina Arnold² Michael S. Arnold³ Larry Lüer⁴ Vasili Perebeinos⁵ Phaedon Avouris⁵ Mark C. Hersam⁶ Manfred Kappes² Guglielmo Lanzani⁷ Department of Physics and Astronomy, Vanderbilt University, Nahville

²Institut für Physikalische Chemie, Universität Karlsruhe, Karlsruhe, Germany

 3 Department of Physics, University of Michigan, MI 48109, USA

⁴National Laboratory for Ultrafast and Ultraintense Optical Science, INFM-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy

 $^5\mathrm{IBM}$ Research Division, T. J. Watson Research Center, Yorktown Heights, New York 10598, USA

⁶Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208-3108, USA

⁷CNISM and Dipartimento di Fisica, Politecnico di Milano, P.za L. da Vinci 32, 20133 Milano, Italy

We discuss recent investigations of several key photophysical properties of Carbon Nanotubes: 1) the decay of the E_{22} resonance [1] 2) the size and 3) the mobility of E_{11} excitons in semiconducting SWNTs [2] and 4) the nonlinear optical response of M_{11} excitons in metallic SWNTs [3]. Some of these investigations have benefited tremendously from recent advances of post synthesis sample preparation techniques [4,5]. Specifically, we find that samples prepared by density gradient ultracentrifugation are free of contaminations from small bundles or ropes of nanotubes which may have affected earlier studies using colloidal nanotube suspensions.

- 1 T. Hertel, V. Perebeinos, J. Crochet, K. Arnold, M. Kappes, and Ph. Avouris, Nano Lett. (in press).
- 2 L. Lüer, S. Hoseinkhani, D. Polli, J. Crochet, T. Hertel, G. Lanzani, (in preparation).
- 3 T. Hertel, Z. Zhu, M.S. Arnold, M.C. Hersam, (in preparation)
- 4 M.S. Arnold, S.I. Stupp and M.C. Hersam, Nano Lett., 5 (2005) 713.
- 5 Crochet, J., M. Clemens, and T. Hertel, J. Am. Chem. Soc., 129 (2007) 8058.

Drift effect on fluctuation enhanced gas sensing

Zoltan Konya¹ Akos Kukovecz¹ Henrik Haspel¹ Imre Kiricsi¹ Radu Ionescu² Robert Mingesz³ Zoltan Gingl³ <u>Peter Heszler</u>⁴ Krisztian Kordás⁵ Niina Halonen⁵ Geza Toth⁵ Jani Maklin⁵ Jouko Vahakangas⁵ Tero Mustonen⁵ Hannu Moilanen⁵

¹Dept. of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary

²Dept. of Electronics, Electrical and Automatic Engineering, Rovira i Virgili University, Tarragona, Spain

³Dept. of Experimental Physics, University of Szeged, Szeged, Hungary

⁴Dept. of Optics and Quantum Electronics, University of Szeged, Szeged, Hungary ⁵Microelectronics and Materials Physics Laboratories, Dept. of Electrical and Information Engineering, University of Oulu, Oulu, Finland

A low-noise electronic system is built and tested for fluctuation enhanced gas sensing (FES). This latter is a new technique and based on the determination of the power spectral density (PSD) of the stationary resistance fluctuations of semiconductor gas sensors. Its use is advantageous for improving the chemical selectivity of the sensors. However, subsequent to an initial fast change, as a sensor is exposed to an analyte gas, a typical drift of the resistance can be observed. This effect hinders evolving stationary conditions and thus acquiring fast measurements when applying FES. Therefore, this drift effect is studied both experimentally and theoretically. PSDs are gathered and simulated numerically with and without drift conditions, the results are compared and lower frequency limits are given for correct use of FES. Functionalized single wall carbon nanotube layers on silicon chips serve as active material for the experimental investigations.

50

Carrier-carrier interaction in single-wall carbon nanotubes: Theory of non-equilibrium and ultrafast nonlinear optical properties

Stephanie Reich 1 Christian Thomsen 2 Matthias Hirtschulz 3 Frank Milde 3 Ermin Malić 3 Andreas Knorr 3

¹Fachbereich Physik, Freie Universität Berlin, Berlin

²Institut für Festkörperphysik, Technische Universität Berlin, Berlin

³Institut für theoretische Physik, Technische Universität Berlin, Berlin

Recent theoretical studies of optical properties of carbon nanotubes (CNTs) are focused on their linear optics including the formation of excitons. Here, we present a carbon nanotube Bloch equation (CNBE) approach in the time domain. The equations reproduce well-known linear excitonic absorption spectra, but extend the theory to non-stationary non-equilibrium situations where carrier-carrier scattering dominates the ultrafast nonlinear response. First, the time dependent Hartree-Fock contributions to the equation of motion for the interband coherence and electron

densities are discussed. We show how our approach predicts band renormalization and excitonic effects. Both contributions lead to a net blue shift of the CNT absorption and reshaping of the optical resonances via exciton formation. Second, we analyze, in a screened Hartree-Fock model, the nonlinear carrier density dynamics and the optical Stark effect of CNTs. We discuss the response of CNTs to an ultrafast pump pulse, treating the non-stationary dynamics of the non-equilibrium CNBEs. Third, we extent the theory beyond the time dependent Hartree-Fock level and take into account electron correlations, in particular electron-electron scattering for highly excited CNTs. The influence of carrier-carrier scattering on nonlinear optical properties of CNTs is discussed.

51

Interface dynamics of crystalline catalysts during Si nanowire and carbon nanotube CVD

S. Hofmann¹ R. Sharma² C. T. Wirth¹ F. Cervantes-Sodi¹ C. Ducati¹ T. Kasama¹ R. Dunin-Borkowski³ J. Drucker² P. Bennett² J. Robertson¹

Self-assembled nanowires and nanotubes offer the prospect of accurate and scalable device engineering at an atomistic scale. However, deterministic nanotube growth and the control of nanowire dopant profiles and heterostructures are limited by an incomplete understanding of the role of commonly used catalysts and specifically their interface dynamics.

Here, we present lattice-resolution, video-rate in-situ transmission electron microscopy studies of the nucleation and growth of Si nanowires for liquid and solid catalyst systems [1]. In both cases, the Si nuclei are initially smaller than the catalyst particles, before expanding and pushing the catalysts onto the tips of the growing wires. For solid catalyst crystals the dominant, coherent nanowire growth interface is observed directly to advance by the lateral propagation of ledges. We propose that interfacial ledge propagation plays a central role in nanowire self-assembly and compare the dynamic catalyst reshaping to graphene nucleation on stepped transition metal films and carbon nanotube formation [2].

- 1 Hofmann S., Sharma R., Wirth C. T., Cervantes-Sodi F., Ducati C., Kasama T., Dunin-Borkowski R., Drucker J., Bennett P., Robertson J., submitted (2007).
- 2 Hofmann S., Sharma R., Ducati C., Du G., Mattevi C., Cepek C., Cantoro M., Pisana S., Parvez A., Ferrari A. C., Dunin-Borkowski R., Lizzit S., Petaccia L., Goldoni A., Robertson J., Nano Lett. 7, 602 (2007).

¹University of Cambridge, Cambridge, UK

²ASU, Tempe, US

³DTU, Copenhagen, Denmark

SILICON CARBIDE NANOWIRES: CHEMICAL CHARACTERIZATION AND MORPHOLOGY

<u>A. Huczko</u>¹ S. Cudzilo² K. Polanski³ W. Olejniczak³ Z. Klusek³ P.J. Kowalczyk³ M. Rogala³ P. Dabrowski³ A. Busiakiewicz³ W. Kozlowski³

¹Department of Chemistry, Warsaw University, 02-093 Warsaw, Poland

 $^2\mathrm{Department}$ of Chemistry, Military University of Technology, 00-980 Warsaw, Poland

³Department of Solid State Physics, University of Lodz, 90-236 Lodz, Poland

Silicon carbide nanowires (SiC NWs) have been efficiently obtained via combustion synthesis route from Si/PTFE mixtures. The protocol of isolation and purification of SiC NWs has been elaborated. We present the results of studies of the morphology of these nanostructures. The SEM investigations were carried out to find out the lengths and diameters of the nanowires (20-100 nm dia. and several microns in length). EDX, XPS and AES were used to investigate the chemical composition of the nanowires. From XPS and AES we found out that the SiC nanowires are nitrogen doped. In addition, the ARXPS results showed that outer regions of the nanowires are carbon rich. These results in conjunction with low resistance of the nanowires suggest that nitrogen dopant and the carbon rich surface are responsible for conducting properties of SiC NWs. Acknowledgement. This work was supported by the Ministry of Education and Science through the Department of Chemistry, Warsaw University, under Grant No. 3 T08D 012 28.

53

Electronic system of graphene probed by Raman spectroscopy

Martin Hulman¹ Miro Haluška² Giusy Scalia³ Dirk Obergfell³ Siegmar Roth³

¹Danubia NanoTech, Bratislava, Slovakia

²Nano and Micro Scale Engineering, TU Eindhoven, Netherlands

³Max-Planck Institut für Festkörperphysik, Stuttgart, Germany

We present the results of the Raman scattering experiments performed on different single-layer graphene samples. The position and the line width of the Raman-active G - band changes as a result of the intentional doping from the environment. From the former, the temperature of the electronic system could be derived. Even for a low laser power, the temperature is significantly higher than the temperature of the sample. On the other hand, the phonon system is not affected and a heating induced down-shift of the G - band was not observed. A low-intensity satellite line was observed in addition to the main peak in the G-band. Unlikely the latter, the position of the satellite is independent of the carrier concentration. We assigned the line due to intraband electronic transitions predicted theoretically.

Singlet-Triplet Physics and Shell Filling in Carbon Nanotube Double Quantum Dots

Henrik Ingerslev Jørgensen¹ Kasper Grove-Rasmussen¹ Poul Erik Lindelof¹ Niels Bohr Institute, Nano-Science Center, Copenhagen University

We have fabricated devices consisting of a nanotube contacted by titanium electrodes, and gated by three narrow local gates. At low temperatures the device behaves as two serially coupled quantum dots, i.e., a double quantum dot, where each quantum dot is tunable by one of the local gates [1-2]. The local gates are fabricated as either top-gates, or as gates underneath the nanotube called trench-gates.

When adding electrons to the nanotube double quantum dot by tuning the local gates we observe that it has a shell structure of either 4 electrons or 8 electrons [2]. We have made magnetic field spectroscopy on one of the 4-electron shells and identified singlet and triplets states. The splitting between the singlet and triplet states, called the exchange energy, is also estimated. Finally, we observe that the singlet and triplet states can mediate inelastic cotunneling.

- 1 H. I. Jørgensen et. al. Appl. Phys. Lett. 89, 232113 (2006).
- 2 H. I. Jørgensen et. al. arXiv:0711.3245

55

Optical properties of individual boron nitride nanotubes

<u>Perine Jaffrennou</u>¹ Julien Barjon² Jean Sebastien Lauret³ Brigitte Attal Tretout⁴ Francois Ducastelle¹ Annick Loiseau¹

Boron nitride nanotubes (BNNT), which were discovered in 1995, are composed of rolled up hexagonal boron nitride (hBN) sheets. According to calculations, they are, as their related bulk material, hBN [1], wide band gap semiconductors and are expected to strongly emit in the UV range [2, 3]. On contrary to carbon nanotubes, it is predicted that their electronic and optical properties should not depend too much on their diameter and helicity. In addition, recent theoretical calculations show that, as it has been experimentally demonstrated for hBN [4, 5], strong excitonic effects should occur in BNNT, with localized excitons of very large binding energy (quasi-Frenkel excitons) [2, 3]. Such effects have not been experimentally demonstrated yet, especially because of a lack of pure BNNT samples.

In our study, cathodoluminescence spectroscopy and imaging on individual BNNT have been undertaken and are compared to photoluminescence and photoluminescence excitation experiments on BNNT macroscopic samples [6, 7]. The results

¹Laboratoire d Etude des Microstructures, ONERA, Chatillon, France

 $^{^2\}mathrm{GEMaC},$ Universite Versailles St
 Quentin, Meudon, France

³LPQM, ENS Cachan, Cachan, France

⁴DMPH, ONERA, Palaiseau, France

confirm that BNNT are strongly UV luminescent materials and that light is emitted all along the nanotube. In order to understand the origin of this UV emission, the spectra are compared to those obtained for the bulk material, hBN. The optical signal of BNNT is composed of two emission bands located in the range of 3 to 6 eV. The far UV luminescence band observed at about $5.3~{\rm eV}$ is attributed to excitonic recombinations and the $3.8~{\rm eV}$ luminescence band is related to impurity centers.

- 1 B. Arnaud et al., Phys. Rev. Lett. 96, 026402 (2006).
- 2 C.-H. Park et al., Phys. Rev. Lett. 96, 126105 (2006).
- 3 L. Wirtz et al., Phys. Rev. Lett. 96, 126104 (2006).
- 4 K. Watanabe et al., Nat. Mat. 3, 404 (2004).
- 5 P. Jaffrennou et al., J. Appl. Phys. 112, 116102 (2007).
- 6 P. Jaffrennou et al., Chem. Phys. Lett. 442, 372 (2007).
- 7 P. Jaffrennou et al., phys. stat. sol. (b) 244, 4147 (2007).

56

Photoluminescence spectroscopy and atomic force microscopy of individual SWNTs

 $\underline{Stefan\text{-}Sven\ Jester}^1$ Oliver Kiowski² Frank Hennrich² Sergei Lebedkin² Ninette Stürzl¹ Kai Moshammer¹ Manfred M. Kappes²

¹Inst. f. Physikalische Chemie Mikroskopischer Systeme, Universität Karlsruhe, Kaierstr. 12, 76128 Karlsruhe, Germany

²Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Photoluminescence microscopy (PL) and atomic force microscopy (AFM) are used to examine individual SWNTs supported on sapphire. The nanotubes can be reproducibly relocated by markers, prepared by electron beam lithography. PL allows the examination of the electronic properties of semiconducting SWNTs. High resolution AFM images provide information about the tube diameter, and allow to distinguish between individual SWNTs and bundles or assemblies. The combination of both experiments results in information about the electronic properties, which do not only depend on the chiral indices (n,m), but also on the local tube environment, and interactions with adjacent tubes. We present a statistics of individual SWNTs and bundles.

The two-peaks Gprime band in carbon nanotubes

<u>Ado Jorio</u>¹ Indhira O. Maciel¹ Marcos A. Pimenta¹ Humberto Terrones² Maruricio Terrones² Apparao M. Rao³

 $^{1}\mathrm{Departamento}$ de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte

²IPICYT, San Luis PotosÃ, MEXICO

³Clemson University, Clemson, USA

In this work we study the effect of defects in the electronic structure of carbon nanotubes using Raman spectroscopy. We study carbon nanotubes grown by laser ablation and chemical vapor deposition (CVD), the last ones known to be more defective. We also study laser ablation and CVD grown doped tubes using B, N and P in the precursor materials. The lower frequency peak of the doublet G' band comes from the defective areas, as shown by near-field Raman and near-field hoto-luminescence experiments. From its frequency dependence on the excitation laser energy, and from the dependence on p vs n doping, we propose the new feature is shifted from the pristine G' due to renormalization of the electron energy.

58

MEMS-enabled Raman thermal imaging of suspended individual SWNTs

Alain Jungen¹ Julius Gauckler¹ Christoph Stampfer² Christofer Hierold¹

Microelectromechanical systems (MEMS) have been used as a particular place-holder for individual single-walled carbon nanotubes (SWNTs) for the study of their properties [1]. Besides presenting an overview of enabling nanoscience through MEMS, we present spatially resolved Raman studies of individual SWNTs. Samples were comprised of microheaters with integrated and suspended SWNTs. We found the phonon frequency to depend on temperature by $d\omega/dT$ =-0.0305 cm⁻¹/K, measured at the G-line Γ-phonon. The highest measured *local* (spotsize of approx. 400 nm) temperature in a SWNT was about 1000 K. Further studies emphasize the effect of temperature on the energy shift of the optical transition energies. By performing spatially resolved line cuts across the tubes, we found a strong off-resonance effect [2] resulting in reduced Raman intensity due to transition energy shifts.

- 1 A. Jungen, S. Hofmann, J. C. Meyer, C. Stampfer, J. Robertson, S. Roth, and C. Hierold, *J. Micromech. Microeng.*, 17 (2007), 603-608.
- 2 A. Jungen, V. N. Popov, C. Stampfer, L. Durrer, S. Stoll, and C. Hierold, *Phys. Rev. B*, 75 (2007), 041405(R).

¹Micro and Nanosystems, ETH Zurich

²Solid State Physics Laboratory, ETH Zurich

Doped and irradiated SWNT networks: what is the origin of the correlation between conductivity and Raman peak frequencies?

Alan B. Kaiser¹ Viera Skakalova²

¹MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington

²Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Despite the different origins of the G, D and D* Raman modes, there is a remarkable correlation between their frequency shifts and changes in the conductivity and Young modulus of freestanding single-wall carbon nanotube (SWNT) networks. On ion irradiation, all these properties show similar peaks as a function of irradiation dose. On acceptor doping that increases conductivity, increases are also observed in the Raman mode frequencies that are closely analogous to the irradiation effects. We discuss the most likely reasons for the correlations between changes in these properties, including a discussion of the conduction mechanisms involved [1] and the effect of thermal annealing due to irradiation on conductivity[2].

- 1 A.B. Kaiser, V. Skakalova and S. Roth, Physica E, to appear (2008).
- 2 V. Skakalova, A.B. Kaiser, Z. Osvath, G. Vertesy, L.P. Biro and S. Roth, Applied Physics A, to appear (2008).

60

The in-situ Raman spectroelectrochemistry of individual SWCNTs

Martin Kalbac¹ Ladislav Kavan¹ Hootan Farhat² Jing Kong² Mildred S. Dressel-

¹J. Heyrovsky Institute of Physical Chemistry, ASCR, Dolejskova 3, CZ-18223 Prague 8, Czech Republic. Tel: 420 2 6605 3804; Fax: 420 2 8658 2307;

²Department of Electrical Engineering and Computer Science, MIT, Cambridge, Massachusetts 02139, USA

The probing of the sensitivity of carbon nanostructures to electrochemical doping gives important information on the structure of these materials. In situ Raman spectroelectrochemistry is a well established method to investigate the behavior of single wall carbon nanotubes (SWCNTs) during doping. We have shown previously that electrochemical doping has a strong impact on the development of the Raman spectra of SWCNT bundles. However the interpretation of these results on bundle samples was extremely difficult. Here we show results on electrochemical doping of individual SWCNTs. We have been able to follow precisely the development of the Raman modes of particular SWCNTs, which significantly simplifies the analysis of the measured data. In general, we have found that the results obtained on individual

SWCNTs are in agreement with those measured on SWCNT bundles. However the magnitude of the effects seems to be specific for SWCNTs with particular (n,m). In extreme cases even opposite trends in development of nanotube modes during the electrochemical charging can be observed. These effects can not be obviously found on SWCNT bundles since such effects are averaged out in summing over the ensemble of tubes and new effects arising from the interaction between tubes must also be considered.

61

Selective adhesion of osteoblasts on differently patterned nanocrystalline diamonds

<u>Marie Kalbacova</u>¹ Lenka Michalikova² Veronika Baresova¹ Alexander Kromka² Bohuslav Rezek² Stanislav Kmoch¹

¹ Institute of Inherited Metabolic Disorders,1st Faculty of Medicine, Charles University, Prague, Czech Republic

²Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

The compatibility of engineered surfaces with tissues, cells and biological molecules is crucial in development of medical diagnostics, biosensors, drug delivery systems, etc. Nanocrystalline diamond (NCD) films represent novel materials, which have superior electro-optical and mechanical properties for such devices (wide band gap up to far UV, 2D surface conductivity, high resistance, stability and wear resistance) and are amendable for selective surface termination, which may ensure optimal conditions for bio-molecules and cell attachment and behavior. In this work, we studied adhesion, growth and viability of human osteoblastic cells on NCD films with the aim to define optimal semiconductor surfaces for novel thin-film biosensor devices. Human osteoblasts (SAOS-2) were cultured on differently patterned and terminated NCD films with alternating H- and O-terminated stripes of different width (30, 100, 200 micrometers) and different patterns like triangles, squares or circles. Cells were seeded at different densities and fluorescently visualized at different time points. We found that cell attachment is guided by the hydrophobic/hydrophilic structures with preferential primary adhesion on O-terminated surfaces. Our observations suggest that the cell adhesion is selectively controlled on thin film electronic device surfaces, through the patterning of hydrophobic/hydrophilic surface coatings.

62

Effect of band structure on field emission

Vsevolod Leonidovich Katkov

Joint Institute for Nuclear Research, University Centre of Joint Institute for Nuclear Research, Dubna

The field emission of crystalline AAA graphite is studied within a simple analy-

tical approach with account of the dispersion relation near the Fermi level. The emission current is calculated for two crystal orientations with respect to the applied electric field. It is found that the exponent of the Fowler-Nordheim equation remains the same while the preexponential factor is markedly modified. For both field directions, the linear field dependence is found in weak fields and the standard quadratic Fowler-Nordheim behavior takes place in strong fields. A strong dependence of the emission current from the interlayer distance is observed. As an illustration of the method the known case of a single-walled carbon nanotube is considered.

63

Novel organometallic surfactant for solubilization of single walled carbon nanotubes: Application for Li-ion batteries

Ladislav Kavan¹ Ivan Exnar² Jiri Cech³ Michael Graetzel⁴

 1 J. Heyrovsky Institute of Physical Chemistry, v.v.i. Dolejskova 3, CZ-18223 Prague 8

²High Power Lithium, SA, PSE-B, Ecublens, CH-1015 Lausanne, Switzerland

³PragueLehigh University, Department of Materials Science and Engineering, 5 East Packer Avenue, Bethlehem, PA 18015, USA

⁴Laboratory of Photonics and Interfaces, EPFL, Ecublens, CH-1015 Lausanne, Switzerland

The amphiphilic Ru-bipyridine complex NaRu(4-carboxylic acid-4*-carboxylate-2,2*-bipyridine)(4,4*-dinonyl-2,2*-bipyridine)(NCS)2 can be used as a surfactant for solubilization of single walled carbon nanotubes (SWNTs). The Ru-complex represents a redox functionality of 3.5 V vs. Li/Li+ anchored to SWNT. Electrodes fabricated from the Ru-complex/SWNT/LiFePO4(olivine) composite exhibited greatly enhanced activity for electrochemical Li extraction/insertion compared to the performance of electrodes made from LiFePO4 derivatized either by adsorption of sole Ru-bipyridine complex or by carbon nanotubes dispersed with the redox inactive pyrene butanoic acid. This so called nanotube wiring effect is based on a synergic action of adsorbed redox-active molecule, which provides the interfacial charge transfer to the olivine surface and the SWNT, which transports charge to longer distances in the composite. The paper will review our initial study of the effect [1], and it will also summarize new results from recent studies of SWNTs of varying diameters. The narrow CVD-grown carbon tubes (CoMoCat) enhance the wiring effect similarly to wider laser-grown tubes, but, interestingly, the narrow tubes improve the activity for anodic wiring more than the laser-grown tubes, and vice versa for cathodic wiring.

1 L. Kavan I. Exnar, J. Cech, M. Graetzel, Chem. Mater. 2007, 19, 4716.

Photoluminescence Excitation Spectroscopy on individual SWNTs: suspended, on a surface and under strain

Yan Li 1 Zhong Jin 1 Oliver Kiowski 2 Sergei Lebedkin 2 M. M. Kappes 2 Stefan-Sven Iester 3

¹Beijing National Laboratory for Molecular Sciences, Key Laboratory for the Physics and Chemistry of Nanodevices, College of Chemistry and Molecular Engineering, Peking University, Bejing 100871, China

²Forschungszentrum Karlsruhe, Institut fuer Nanotechnologie, 76021 Karlsruhe, Germany

³Universitaet Karlsruhe, Institut fuer Physikalische Chemie, Lehrstuhl fuer die Physikalische Chemie Mikroskopischer Systeme, 76128 Karlsruhe, Germany

Photoluminescence-excitation (PLE) spectroscopy was applied to ultra-long individual single-walled carbon nanotubes (SWNTs), directly CVD-grown on Si/SiO2 substrates. Due to etched trenches in the substrate, we are able to detect changes in PL (relative quantum yield, shifts in optical transition energies E11 and E22, FWHM of E11 emission and E22 excitation) between suspended and unsuspended parts of individual SWNTs and up to 600 micrometer along a nanotube using PLE spectroscopy with a home-built PL microscope.

We also applied uniaxial and torsional strain to individual SWNTs on the surface via AFM manipulation. E11/E22 variations due to uniaxial strain follow the well-known family pattern related to $\mathbf{q}=(\mathbf{n}\text{-}\mathbf{m})\mathbf{mod}$ 3 whereas for torsional strain E11 and E22 increase for both $\mathbf{q}=1$ and -1. The propagation range of uniaxial strain is approx. 100 microns and hence a lot larger than torsional strain with approx. 10 microns, in agreement with the results of Liu and Kong et al.[1, 2] However, we find an abrupt return to the unstrained SWNT as opposed to a continuous relaxation found by Liu and Kong et al.

Apart form shifts in E11 and E22 we also present variations in relative quantum yield and FWHM along strained SWNTs.

- 1 Xiaojie Duan et al, Nano Letters 7, 2116 (2007).
- 2 Bo Gao et al, Nano Letters **7**, 750, (2007).

65

Raman spectroscopy of isolated double walled carbon nanotubes

<u>Kenji KISODA</u>¹ Toshiya Murakami² Ryoji Naito² Kazuyo Matsumoto² Hitoshi Kakehi² Hiroshi Harima²

We have studied isolated double walled carbon nanotube (DWCNT) by Raman spectroscopy. After isolation procedure, clustered lines of radial breathing ${\rm mode}({\rm RBM})$

¹Wakayama University, Wakayama, Japan

²Kyoto Institute of Technology, Kyoto, Japan

dissapeared. Instead, a sharp RBM peak emerged. The peak frequency changed with different outer tube diameters. The unusual behaviour of the G band was explained by the resonance enhancement of the outer tubes.

66

FIELD EMISSION from SINGLE-WALL CARBON NANOTUBES SYNTHESIZED from C:BN MIXTURES

 $\underline{\text{V.I. Kleshch}}^1$ E.D. Obraztsova
 1 N.R. Arutyunyan 1 V.V. Grebenyukov
 2 A.S. Pozharov 1 A.N. Obraztsov
 2

¹A.M. Prokhorov General Physics Institute RAS, Moscow, Russia

Theoretical study of C:BN heterophase nanotubes predicts a possibility to change their bandgap depending on the amount of BN inclusions into the carbon nanotube walls. Such materials with a controllable bandgap are demanded for many applications (vacuum electronics, laser physics etc.) We used arc-discharge technique to embed hexagonal boron nitride (h-BN) into single-wall carbon nanotubes (CSWNTs). We started from the optimal synthesis conditions of CSWNTs and than partially (up to 50%) replaced the graphite fraction by h-BN powder in the anode filling. According to the Raman data single-wall nanotubes were synthesized in all cases. We report here the study of field emission properties of the materials obtained. Experiments were held in a vacuum diode system consisting of a cathode formed from a raw soot and a plane anode mounted in a vacuum chamber. Current-voltage characteristics of our samples have shown the emission threshold field lowering with the BN percentage increasing. A slope of the Fowler-Nordheim dependence has been found to increase proportionally to BN concentration. Besides for the samples grown from C:BN mixtures the Fowler-Nordheim plots demonstrated a non-linear behavior at high fields. These results may be interpreted as an indirect evidence of the BN embedding into the carbon nanotube walls. The work is supported by FP6, INTAS and RAS projects.

67

Phonon dispersion of small diameter semiconducting chiral carbon nanotubes - a theoretical study

<u>János Koltai</u>¹ Viktor Zólyomi² Jenő Kürti¹

Significant changes in the phonon dispersion of single walled carbon nanotubes with decreasing diameter have been observed experimentally. We present first principles calculations on the phonon dispersion of a large number of small diameter semiconducting chiral single walled carbon nanotubes. The use of density functional

²Department of Physics, Moscow State University, Russia

¹Department of Biological Physics, Eötvös University Budapest, Budapest

²Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Budapest

theory for unit cells containing hundreds of atoms was only possible because the helical symmetry was taken into account explicitly in our calculations. The results can be useful for interpretation of experiments, especially on CoMoCat tubes, but also on HiPCo tubes and the inner walls of double walled carbon nanotubes. The phonon dispersion of several larger diameter tubes have also been calculated for comparison. A clear phonon softening with decreasing diameter can be observed.

68

TEM imaging of organic molecules in motion in/on CNT

Masanori Koshino¹ Kazutomo Suenaga² Eiichi Nakamura¹

¹ERATO, JST, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

²Research Centre for Advanced Carbon Materials, National Institute of Advanced Industrial Science and Technology (AIST), Higashi, Tsukuba, Ibaraki 305-8565, Japan

We report herein the observation of a single small organic molecule either at rest or in motion interacting with a single wall carbon nanotube (CNT), with near-atomic resolution. Hydrocarbon chains, aromatic rings, amide bond, and other fundamental groups in biology connected with a carborane or C_{60} fullerene tags are visualized during their movements by transmission electron microscopy (TEM), despite the assumed high sensitivity of organic molecules to damage by electron impact, which has discouraged previous explorations of the imaging. The effects of external temperature, electron irradiation, inside or outside of CNT on the observations are discussed based on the TEM observations of accelerationg voltage of 120 kV at 293 K and 4K.

69

Linear plasmon dispersion in single wall carbon and the excitation spectrum of graphene

<u>Christian Kramberger</u>¹ Thomas Pichler¹ Ralf Hambach² Lucia Reinning² Erik Einarsson³ Shigeo Maruyama³

We have measured a strictly linear π plasmon dispersion along the axis of individualized single wall carbon nanotubes, which is completely different from plasmon dispersions of graphite or bundled single wall carbon nanotubes. Comparative ab initio studies on graphene based systems allow us to reproduce the different dispersions. This suggests that individualized nanotubes provide viable experimental access to the fundamental electronic excitations of graphene, and it validates the use of graphene to understand electronic excitations of carbon nanotubes. In particular, the calculations reveal that depolarization effects cause a mixing of electronic

¹IFW Dresden, Germany

²Ecole Polytechnique, Palaiseau, France

³Univ. Tokyo, Dept Mech Engn, Japan

transitions, including the 'Dirac cone', resulting in the observed linear dispersion.

70

Ion energy influence on the carbon nanostructuring in C:Ni nanocomposite films

 $\underline{\mathrm{M.\ Krause}^1}$ L. Ryves 2 M. M. M. Bilek 2 G. Abrasonis 1 F. Munnik 1 M. Berndt 1 A. Kolitsch 1 W. Moeller 1

 $^{1}\mbox{Institute}$ of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, Dresden

Nanocomposites are heterogeneous materials wherein the lateral extension of at

²School of Physics, The University of Sydney

least one component is lower than 100 nm.[1] They are advanced functional materials whose structural, electronic, and mechanical properties cannot be predicted from the properties of their constituents alone. This is partially due to the presence of interfaces, which occupy a considerable volume fraction of the nanocomposites. Nanocomposites, comprised of metallic nano-particles embedded in a carbon matrix have recently attracted considerable attention, [2]-[4] due to their promising mechanical, optical and magnetic properties. Despite many studies, the mechanisms responsible for the nanostructuring of both constituents are not well understood. In this study, the influence of the energy of the depositing species in the C:Ni system is investigated. This is achieved by the comparison of the C:Ni film structures grown by ion beam sputtering (IBS) and pulsed filtered cathodic vacuum arc (PFCVA) deposition. The films studied were deposited with substrate temperature in the range (RT-500C) and with Ni contents of 8 at%, 15 at%, and 30 at%. The main difference between the two growth methods is the energy distribution of depositing species which is 1-10 eV for IBS and 100 eV PFCVA. The higher ion energy allows the synthesis of hydrogen free tetrahedral amorphous carbon (ta-C) in Ni-free films. Structural properties of the films were analysed by XRD and wavelength dependent Raman spectroscopy. The structures observed for nickel were correlated with the growth temperature and the nickel concentration and included a low-crystalline, a hexagonal and a fcc phase. Independent of its crystalline structure, Ni catalyses the formation and the long-range ordering of 6-fold aromatic ring structures in the carbon phase. This effect was observed in films deposited by both methods. The higher energy in PFCVA appears to counteract the ordering process, as indicated by the lower I(D)/ I(G) Raman line intensity ratio and by the smaller splitting of carbon D- and G-line compared to IBS grown C:Ni thin films. The higher incoming energy flux also enhanced the formation of new carbon structures with Raman spectroscopic features at 550 and 1100 cm-1 both of which showing a resonance enhancement for visible laser excitation.

1 P. M. Ajayan, L.S. Schadler, P.V. Braun, Nanocomposites Science and Technology, Wiley, (2005).

- 2 T. Hayashi et al., Nature 381, 772-774 (1996).
- 3 C. Guerretpiecourt et al., Nature 372, 761-765 (1994).
- 4 M. Krause et al., Phys. Stat. Sol. (B), 244, 4236-4239 (2007); G. Abrasonis et al., Carbon, 45, 2995-3006 (2007).

Low impedance multi-wall carbon nanotube films made suitable for temperature and pressure measurement by localized charge injection

<u>Akos Kukovecz</u>¹ Rita Smajda¹ Mariann Oze¹ Balazs Schaeffer¹ Henrik Haspel¹ Zoltan Konya¹ Imre Kiricsi¹

¹Dept. of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary

Self-supporting mats of multi-wall carbon nanotubes (MWCNT buckypaper) are an interesting and versatile nanotube application platform. In the course of our explorations in this field we prepared MWCNT buckypapers with a surface density of 5.6 mg/cm2 and modified their surface with pyroelectric LiNbO3 and piezoelectric KNbO3 crystals. The temperature and pressure sensitivity of the prepared devices was larger than that of the undoped buckypapers. A possible explanation for this phenomenon is that the dopant crystals act as localized charge injection points influencing the conduction paths in the buckypaper. We believe that the described method opens a new path for buckypaper functionalization.

72

Infrared microreflectance study of magnetically aligned single-wall carbon nanotubes under pressure

C. A. Kuntscher¹ K. Thirunavukkuarasu¹ K. Kamaras² F. Simon³

¹Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany

 $^2{\rm Research}$ Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O.Box 49, H-1525 Budapest, Hungary

³Budapest University of Technology and Economics, Institute of Physics and Solids in Magnetic Fields Research Group, Hungarian Academy of Sciences, P.O. Box 91, H-1521 Budapest, Hungary; University of Vienna, Faculty of Physics, Strudelhofgasse 4, A-1090 Wien, Austria

We report on the pressure-dependent optical response of single-wall carbon nanotube networks (buckypapers) aligned in a magnetic field. The degree of orientation of the tubes in the buckypaper was about 70%. By measuring the polarization-dependent microreflectance spectra from the far-infrared up to the visible frequency range we wanted to find out about how the anisotropy of the buckypaper changes under pressure. Furthermore, our goal was to find signatures of a pressure-induced

structural phase transition and to study the effect of intertube interaction on the optical response.

The shift of the electronic excitations with pressure shows an anomaly at around 2.7 GPa which we attribute to a structural phase transition. This transition pressure is higher compared to earlier studies on various carbon nanotube materials. Furthermore, the anisotropy in the optical response is preserved up to the highest measured pressure (7 GPa), suggesting that the influence of intertube interaction on the transport properties is small.

Supported by the DFG. Provision of beamtime at the ANKA Angströmquelle Karlsruhe is acknowledged.

73

Conductive, capacitive and visco-elasitic properties of a new composite of the C60-Pd conducting polymer and single-wall carbon nanotubes

<u>Wlodzimierz Kutner</u>¹ Piotr Pieta¹ Emilia Grodzka² Ganesh M. Venukadasula³ Krzysztof Winkler² Francis DSouza³

¹Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw

²Institute of Chemistry, University of Bialystok, Pilsudskiego 11/4, 15-399 Bialystok, Poland

³Department of Chemistry, Wichita State University, Wichita, Kansas 67260, USA

A thin film of a new composite consisting of the redox conductive C60-Pd polymer and single-wall carbon nanotubes non-covalently functionalized with 1-pyrenebutiric acid, (pyr-SWCNTs), was electrochemically prepared in acetonitrile:toluene (1:4, v:v) or o-dichlorobenzene containing C₆₀, pyr-SWCNTs, and Pd acetate under multi-scan cyclic voltammetry (CV) conditions. A 0.1 M (TBA)ClO₄ or (TBA)PF₆ solution was used as the supporting electrolyte. Conductive, capacitive and viscoelasitic properties of the composite were examined by CV and electrochemical impedance spectroscopy (EIS). The observed Raman peaks, characteristic for both pyr-SWCNTs (radial breathing modes, RBM) and C₆₀-Pd, confirmed incorporation of pyr-SWCNTs into the film. The RBM peaks for the pyr-SWCNTs film were deconvoluted in the spectrum of the composite presumably due to diverse aggregation of pyr-SWCNTs. Mass of the deposited composite film was measured in situ by piezoelectric microgravimetry with the use of an electrochemical quartz crystal microbalance. A quartz crystal resonator with its electrode coated by either the C60-Pd or composite film was transferred to a blank supporting electrolyte solution and the current, resonance frequency changes, and dynamic resistance changes vs. potential were simultaneously recorded in different potential ranges. Both films revealed electrochemical activity at potentials more negative than ca. -0.7 V. Both cathodic and anodic currents for the composite film were almost twice as high as those for the C60-Pd films. The presence of pyr-SWCNTs in the film resulted in its higher capacitance. For potentials exceeding -1.2 V, both changes of resonant frequency and dynamic resistance, recorded during the negative potential excursion, were three times smaller for the composite film than those for the C_{60} -Pd film indicating that the former film is more rigid. Redox conductivity of the composite film (14.8 \times 10⁻⁵ S) was higher than that of the C60-Pd film (9.2 \times 10⁻⁵ S). The EIS measurements for different negative potentials revealed capacitive nature of the C_{60} -Pd film and both conductive and capacitive nature of the composite film.

74

Tunable electromagnetic response in onion-like carbon based materials

<u>Vladimir L. Kuznetsov</u>¹ Sergey I. Moseenkov¹ Olga V. Ruhavets² Aleksander V. Gusinski² Arcadii V. Ischenko¹ Polina P. Kuzhir³ Sergey A. Maksimenko³ Olga A. Shenderova⁴ Anatoly I. Romanenko⁵ Timofey I. Buryakov⁵ Olga B. Anikeeva⁵

¹Boreskov Institute of Catalysis, Novosibirsk, Russia

Nanocarbons have potential applications as electromagnetic radiation absorbing and shielding materials. The first results of the microwave (MW) characterization in S-, X- and Ka-bands of onion-like carbon powders (OLC) and OLC-polymer films presented in [1-4] demonstrate high attenuation of a variety of nanocarbon materials over the wide MW frequency range. Here we present the results on the electromagnetic response of OLC of variable composition in Ka-band range (26-37 GHz) combined with measurements of temperature dependence of conductivity.

Controllable graphitization in vacuum of the explosive nanodiamond (ND, d 4-5 nm) within the temperature range 1200-1900 K allows to produce the diamondnanographite composites. As annealing temperature is increased the ratio between diamond core and outer defective curved graphitic shells (sp2-sp3 nanocomposites) decreases, finally resulting in OLC structure. Due to the aggregation of primary ND its annealing products (OLC particles) are organized into aggregates with joint defective graphene shells covering several primary OLC cores. The observed one dimensional variable range hopping conductivity of OLC powders (measured at 4-300 K) combined with HR TEM structural analysis was attributed to the formation of continues ribbon-like defective graphene. The increase of ND annealing temperature results in the increase of density of states of conductive electrons and corresponding increase of conductivity of OLC produced. It was found that conductivity data correlates with EM response of OLC in 26-37.5 GHz range. So the increase of conductivity of OLC results in the increase of EM wave attenuation ability because of growing reflectance ability. Thus the variation of the composition of OLC allows producing materials with controllable EM response.

Acknowledgements: The work was partially supported by the NATO Science for Peace program (grant SfP-981051), INTAS (grant 06-1000013-9225), the State Committee for Science and Technology of Belarus and INTAS (grants 03-50-4409), the

²Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus

³Institute for Nuclear Problem of Belarus State University, Minsk, Belarus

⁴International Technology Center, Raleigh, USA

⁵Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia,

the Belarus Foundation for Basic Research (grant F06R-091), the Russian Foundation for Basic Research (06-03-81038).

- 1 S.A. Maksimenko et al., Diamond and Related Materials (2007) v.16, 1231.
- 2 S.A. Maksimenko et al., Proc. of Metamaterials 2007, Rome, Oct. 2007, pp 903.
- 3 O.Shenderova et al., Diamond and Related Materials (2007).
- 4 J.Macutkevic et.al., Diamond and Related Materials (Ref. No.: DIAM2007 0157).

75

Theoretical study of the electronic band structure and the totally symmetric vibrations of selected CoMoCat carbon nanotubes

Jenő Kürti¹ János Koltai¹ Viktor Zólyomi²

¹Department of Biological Physics, Eötvös University Budapest, Budapest

In situ Raman spectroelectrochemical studies of CoMoCat single-walled carbon nanotubes enriched in (6,5) tubes have been carried out recently. We performed calculations on the density functional theory level using local density approximation for the electronic and vibronic properties of the most abundant tubes in the samples. The following chiral semiconducting tubes were investigated: (6,4), (7,3), (6,5), (9,1), (8,3) and (7,5). The calculated and the measured frequencies of the RBM and G^- modes agree within several wave numbers. The calculated E_{11} , E_{22} transition energies -after 30% upscaling- are comparable with the experimental values. The quenching of the RBM band with p- and n-doping can be interpreted within the rigid band approximation. The validity of the rigid band approximation was shown by calculating the density of states for neutral and charged tubes.

76

Electronic structure of hexagonal and non-hexagonal carbon surfaces Istvan Laszlo

Institute of Physics, Budapest University of Technology and Economics, Budapest

We call a carbon structure carbon surface if the carbon atoms can be imagined being on a 2-dimensional surface. Thus the simplest carbon surface is the graphene sheet. The fullerenes, nanotubes, nanotube junctions and networks of nanotubes are curved graphene sheets. 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

²Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Budapest

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 account. The electronic structure is modified also by possible non hexagonal polygons in the hexagonal network. Here we shall present a simple one orbital one site Hamiltonian for the study of the electronic structure of curved surfaces. The hybridization and the effect of the non-hexagonal polygons is included in the parametrization of the method.

77

Phase Coherent Transport in Graphene Devices

Chun Ning (Jeanie) Lau University of California, Riverside, riverside

We experimentally investigate electronic transport in graphene devices at low temperatures, including supercurrent in graphene devices and quantum hall effect in graphene p-n junctions.

78

Atomic and electronic structure of few layer graphene on SiC(0001) studied with scanning tunneling microscopy and spectroscopy

<u>Peter Lauffer</u>¹ Konstantin V. Emtsev¹ Ralf Graupner¹ Thomas Seyller¹ Lothar Ley¹

¹Technische Physik, Universität Erlangen, Deutschland

Epitaxial growth of graphene on SiC surfaces by solid state graphitization is a promising route for future development of graphene based electronics. In the present work we study the morphology, atomic scale structure, and electronic structure of thin films of few-layer graphene (FLG) on SiC(0001) by scanning tunneling microscopy (STM) and spectroscopy (STS). First we discuss how a quantitative evaluation of the roughness induced by the SiC interface layer can serve as a means to determine the numbers of graphene layers. STS spectra of 2, 3, and 4 ML thick FLG films exhibit characteristic structures that are interpreted in terms of a simple tight binding model [1] which includes a layer dependent potential that is induced by charge transfer from the SiC substrate. Spatially resolved STS measurements on bilayer graphene indicate a local variation of the charge distribution. This is of obvious importance for transport properties and for the question of a substrate induced band gap opening. In addition, we investigate adsorbed PTCDA, a promising organic semiconductor candidate, on FLG surfaces of different thicknesses at liquid helium temperatures. The arrangement of these molecules on graphene is studied and the electronic interaction with the underlying FLG substrate is investigated by tunnelling spectroscopy.

1 Ohta et al., PRL 98, 206802 (2007)

Single-beam pumped Coherent anti-Stokes Raman Scattering on carbon nanotubes

 $\underline{\text{Serge LEFRANT}}^1$ Jean-Pierre BUISSON^1 Jean-Yves MEVELLEC^1 Ioan BALTOG^2 Mihaela BAIBARAC^2

¹Institut des materiaux Jean Rouxel, University of Nantes, Nantes, France

Giant optical fields locally generated in nanoscale metal structures through the local excitation of surface plasmons underlie a variety of nonlinear optical processes. Using silver and gold rough metallic films, reproducible enhancements of the Raman signal on various materials including carbon nanotubes have been demonstrated . In addition, an abnormal anti-Stokes Raman emission, reminiscent of Coherent anti-Stokes Raman Scattering (CARS), is accurately observed on nanometric thin films. We demonstrate that under a tight focusing of the excitation light, a CARS emission, resulting from a wave mixing process between the incident laser light and Stokes Raman light generated by a SERS mechanism, is produced. The results which corroborate the CARS emission are the following: a square relation between the CARS signal intensity and the film thickness; a square relationship between the CARS signal intensity and the exciting laser intensity; a dependence of the CARS intensity on the numerical aperture (NA) of the microscope objective used for the detection of the anti-Stokes signal; a polarization ratio in the anti-Stokes side always greater in comparison with that measured for an usual Stokes Raman signal. We demonstrate also that this mechanism may contribute to a clear identification of the state of the observed nanotubes, i.e. in isolated or bundled forms.

80

INFLUENCE OF EXTRUSION CONDITIONS ON THE IN-LINE MEASURED ELECTRICAL CONDUCTIVITY OF POLYMER-MULTIWALLED CARBON NANOTUBE COMPOSITES

Dirk Lellinger¹ Martin Engel¹ Ingo Alig¹ Petra Pötschke²

In recent years, the applications of polymer - carbon nanotube (CNT) composites have grown rapidly. Although, first polymer-CNT composites are commercially available, a major restraint in market acceptance is the wide variation in electrical conductivity as a function of the processing conditions. In order to study the influence of extrusion conditions on electrical properties experiments have been performed in a slit die flanged to the outlet of a twin screw extruder. The measurement slit die contains two electrodes in plate-plate geometry. AC conductivity and the related complex permittivity were measured in the frequency range bet-

²National Institute of Materials Physics, Bucharest, Romania

¹Deutsches Kunststoff-Institut, Darmstadt

²Leibniz-Institut für Polymerforschung Dresden e.V.

ween 20 Hz and 1 MHz for different extrusion conditions (melt temperature, screw speed, throughput etc.) and after stopping the extruder. The investigations have been performed during melt processing of polycarbonate (PC) and polyamid-6 (PA6) containing 0.5 - 2 wt% and 0.7 - 2.7 wt% of multi-walled carbon nanotubes (MWNT), respectively, for different processing temperatures. During extrusion the conductivity in all samples was found to be comparable to that of the polymer matrix. After the extruder was stopped (model experiment for injection moulding) the conductivity shows a tremendous increase with time (conductivity recovery after shearing). This process was more pronounced for samples with CNT content close to the percolation threshold. The finding can be explained by the reorganization of the conducting network-like filler structure which was (at least partially) destroyed under shear. The reformation kinetics of filler clusters is due to a cooperative aggregation, which is related to the kinetics of cluster-cluster aggregation in a percolating system.

81 Sulfonated Poly(ether ether ketone) Chains Grafted on Carbon Nanotubes Surface

<u>Vincent Leon</u>¹ Moulay-Rachid Babaa² Jean-Louis Bantignies¹ LCVN, Université Montpellier II, Montpellier, France ²CEA-Saclay, France

Among many extraordinary properties, CNTs have a very high Young's modulus, generally reported with a value of 1 TPa, making this kind of material even stronger than diamond and carbon fiber. Moreover their very light weight makes them first choice materials for mechanical reinforcement of polymer matrices. Most of previous studies using CNTs deal with so-called physical mixing, meaning that there is no strong link between polymer and nanotube surface, resulting in a relatively poor enhancement of the composite Young's modulus. In our study, we first investigated the functionalization of multi-walled carbon nanotubes (MWNTs) surface by sulfonated poly(ether ether ketone) SPEEK chains using a direct attachment reaction, PEEK being known as a very promising polymer especially in aerospace field for its particularly high glass transition and melting temperature, compared with most of polymer material. MWNTs were oxidized by a nitric acid treatment to generate carboxyl groups on their surface, which then react with sulfonated groups of SPEEK using hexane diamine as an interlinking molecule. Evidence of covalent functionalization of MWNTs by SPEEK macromolecules was given by near-edge Xray absorption fine structure spectroscopy (NEXAFS) at the C K-edge, O K-edge, and N K-edge and X-ray photoelectron spectroscopy (XPS). Mechanical properties of the MWNT-SPEEK composite material were then tested to quantify the enhancement of Young's modulus.

In-situ Observation on Raman Spectra and Transport Properties of Isolated Single-Wall Carbon Nanotubes

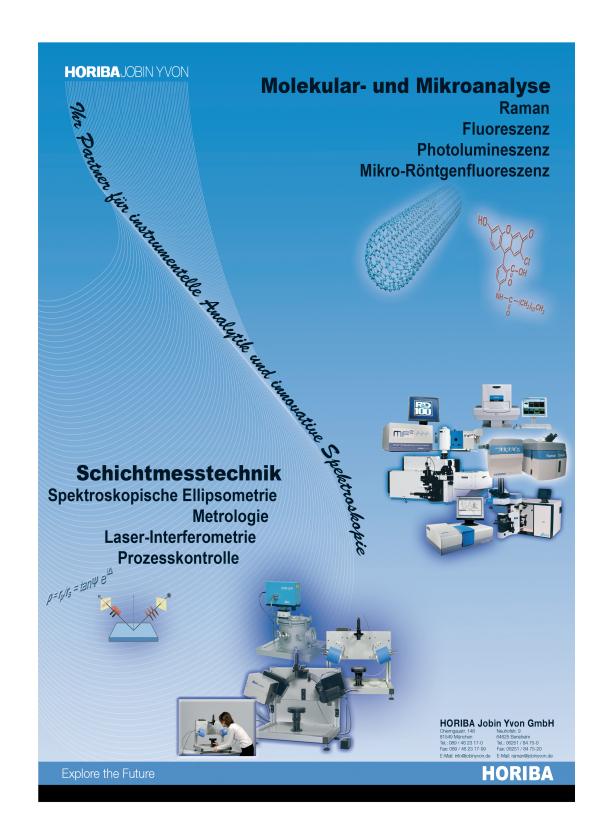
<u>Chen-Wei Liang</u>¹ Wei-Yang Lee² Siegmar Roth¹ Cheun-Horng Tsai²

Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Electrons, when transported in single-wall carbon nanotubes (SWNTs), are scattered by phonons due to electron-phonon coupling (EPC). Such scattering is dominated by different modes of phonons, i.e. acoustic phonons or optical phonons, at different bias range. Modifications of transport properties of SWNTs after applying high bias have been observed and the mechanism is attributed to gas desorption resulting from high-energy phonons due to EPC. To understand the details of the high-field transport and its influence on gas desorption of SWNTs, we conducted an experiment to combine micro-Raman spectra and electrical transport of SWNTs. Results show that the electrical transport generate little effect on Raman shift. This implicates the non-equilibrium state of the phonon induced by EPC. The experimental details and data will be discussed in the presentation.

 $^{^2{\}mbox{Department}}$ of Engineering and System Science, National Tsing Hua University, HsingChu, Taiwan

Poster session Tuesday, March 4



8:30 - 9:00 9:00 - 9:30 9:30 - 10:00	A. K. Zettl, US Catching Waves and Particles With Nanoscale Resonators A. Loiseau, FR Understanding the formation of C-SWNT via in situ and ex situ diagnostics in laser vaporization and CVD techniques D. Mihailovic, SI $Mo_6S_{9-x}I_x$ Nanowire Recognitive Molecular-Scale Connecti- vity: On the Road to Large-Scale Molecular Electronics
10:00 - 10:30	Coffee break
10:30 – 11:00	A. Khlobystov, UK Functionalised Fullerenes in Carbon Nanotubes: Controlled Assembly of Molecular Chains
11:00 – 11:30	A. Hirsch, DE Chemical Functionalization of Fullerenes and CNTs
11:30 – 12:00	U. Kaiser, DE Study of Nano-Carbons by Aberration Corrected Low Voltage Electron Microscopy.
12:30 - 17:00 17:00 - 18:30	Mini Workshops Dinner
18:30 – 19:00	X. Bao, CN Catalysis Chemistry of the Confined Nano-Systems
19:00 – 19:30	A. Minett, AU Modification of CNT Architectures for Alternative Energy Applications
19:30 – 20:00	J. Fischer, US Gallium Nitride Nanowires: Impurity and Disorder Effects on Thermal Conductivity
20:00 – 20:30	A. Tausenev, RU Mode-locked 177-fs soliton erbium-doped fiber laser based on a cellulose polymer film containing SWCNTs synthesized by the arc-discharge method

Non-carbon materials, Fullerenes, DWNT

Wednesday, March 5

8:30

Catching Waves and Particles With Nanoscale Resonators

Alex K Zettl

Department of Physics, University of California at Berkeley, Berkeley, CA 94720 U.S.A.

Nanoscale systems are of interest from both basic science and novel applications viewpoints. In particular, nanoscale mechanical resonators, as might be formed from thin membranes, nanowires, or nanotubes, could exploit novel physics in the interaction of EM waves or atoms and molecules with solids. I will describe work being pursued in Berkeley in using vibrating carbon nanotubes as detectors of radio-frequency EM radiation, as well as them as fully integrated circuit elements for performing rf amplification and decoding functions. Similar geometries may be useful for detection of other system perturbations, including adsorbed atomic and molecular species. The fundamental limits of such transduction systems will be discussed for the different applications.

9:00

Understanding the formation of C-SWNT via in situ and ex situ diagnostics in laser vaporization and CVD techniques

 $\underline{Annick\ Loiseau}^1$ Michèle Cau^2 Marie-Faith Fiawoo^1 Nelly Dorval^2 Jean-Lou Cochon^2 Anne-Marie Bonnot^3 Brigitte Attal-Tretout^2

¹ONERA, BP 72, LEM, UMR 104-CNRS-ONERA, Chatillon

²ONERA, Chemin de la Hunière, 91761 Palaiseau, France

This talk will review on the experimental approaches we have developped at LEM and at ONERA for understanding the formation mechanism of C-SWNT and the role of the chemical nature of the catalyst in both high temperature and CVD techniques.

Concerning high temperature techniques, we have developed a dedicated synthesis reactor based on the continuous laser vaporization of a metal-graphite target and performed various in situ optical diagnostics, using Coherent Anti-Stoke Raman Scattering, Laser Induced Fluorescence and Laser Induced Incandescence to probe vapour and condensed phases involving the carbon soot [1]. The results validate the phenomenological VLS model proposed previously on the basis of TEM analyses of the soot [2] and provide a very comprehensive and quantitative picture of the synthesis process. They reveal the dramatic effect of the metal catalyst on both size and time evolution of the carbon agregates, which has been studied in detail and evidence for the first time the nanotube onset which is found to arise once the condensation of the metal vapour into liquid particles is achieved [3]. Futhermore the results show, by comparing two metal catalysts, Ni and Co, how the nature of the catalyst influences the carbon condensation and the nanotube formation.

³Institut Neel, CNRS-UJF, BP166, 38042 Grenoble, France

Concerning CVD techniques, our approach has consisted to study, by TEM, the evolution of the nanotube nucleation and growth and of the metal particles as a function of the synthesis time and to perform a statistical analysis of the structural and chemical relationships between nanotubes and particles and their substrate. We will show that this approach is very complementary to in situ TEM observations of the nucleation developed recently, and reveal different nucleation mechanisms which will be discussed as a function of both metal and substrate.

- 1 M. Cau, N. Dorval, B. Cao, B. Attal-Tretout, J.L. Cochon, A. Loiseau, S. Farhat, and C.D. Scott. Journal of Nanosciences and Nanotechnology, vol. 6, 2006, p1-11
- 2 J. Gavillet et al, Phys. Rev. Lett. vol 87, 275504, 2001
- 3 M. Cau, N. Dorval, J.L. Cochon, A. Foutel-Richard, C.D. Scott, B. Attal-Tretout, A. Loiseau, Carbon submitted 2008

9:30

${\sf Mo}_6{\sf S}_{9-x}{\sf I}_x$ Nanowire Recognitive Molecular-Scale Connectivity: On the Road to Large-Scale Molecular Electronics

Dragan Mihailovic

Jozef Stefan Institute, University of Ljubljana, Ljubljana

We report on a new highly reproducible route to recognitive self-assembly of molecular-scale circuits using sulfur-terminated subnanometer diameter $Mo_6S_{9-x}I_x$ (MoSIx) molecular nanowires. We demonstrate solution-processed attachment of MoSIx connecting leads to gold nanoparticles (GNPs). We also show that naked nanowires have the potential to bind thiolated proteins such as green fluorescent protein directly, thus providing a universal construct to which almost any protein could be attached. We further demonstrate three-terminal branched circuits with GNPs, opening a self-assembly route to multiscale complex molecular-scale architectures at the single-molecule level.

10:30

Functionalised Fullerenes in Carbon Nanotubes: Controlled Assembly of Molecular Chains

Thomas W. Chamberlain¹ Rudolf Pfeiffer² Herwig Peterlik² Hans Kuzmany² Francesco Zerbetto³ Manuel Melle-Franco³ Luke Staddon¹ Neil R. Champness¹ G. Andrew D. Briggs⁴ Andrei N. Khlobystov¹

Due to their tubular nature, carbon nanotubes (NTs) have been demonstrated to encapsulate different molecules, thus forming quasi one-dimensional molecular systems. Provided that the mechanisms of interactions between the molecules and nanotubes are understood, nanotubes could be used to template formation of molecular chains of desired structure and properties. Previously it has been demonstrated that the most important parameter defining the efficiency of the NT-molecule interaction is the nanotube internal diameter. For example, for spheroidal molecules, such as C60, the nanotube diameter controls the packing arrangement of the molecules. For ellipsoidal C70 or other higher fullerenes the nanotube diameter also controls the orientations of molecules.

An alternative mechanism for controlling the assembly of molecular arrays in NTs is via the size and geometry of functional groups of the molecules inserted in nanotubes. We have synthesised a series of fullerenes functionalised with alkyl- or aryl-groups of various length, width and conformational rigidity to explore this effect systematically. We have inserted these molecules into nanotubes under mild conditions to prevent decomposition of the molecules and to form C60X@NT structures (where X is a functional group). The molecular chains thus formed have been studied by high resolution TEM, XRD, and Raman spectroscopy revealing that the functional groups increase the inter-fullerene separation proportionally with the size of X. However, the functional groups themselves appear to adopt various conformations (as in the case of X = alkyl) or different orientations with respect of each other (as in the case of X = aryl). All these effects create a distribution of inter-fullerene separations in NTs. Our experimental observations are discussed in terms of molecular geometries and inter-molecular interactions and compared with theoretical simulations carried out for these systems.

Acknowledgement: this work is supported by a EUROCORES Programme on Fundamentals of Nanoelectronics (IMPRESS project).

¹School of Chemistry, University of Nottingham, Nottingham NG7 2RD, UK

²Fakultat fur Physik, Universitat Wien, Austria

³Dipartimento di Chimica

⁴Department of Materials, University of Oxford, Oxford OX1 3PH, UK

11:00

Chemical Functionalization of Fullerenes and Carbon Nanotubes

Andreas Hirsch

Department of Chemistry and Pharmacy, Erlangen, Erlangen

andreas.hirsch@chemie.uni-erlangen.de

Fullerenes and carbon nanotubes represent new families of molecular and macromolecular carbon allotropes with unprecedented properties. In order to further modify such properties and in particular to combine them with those of other compound classes chemical functionalization such as, for example, the addition of organic functional molecules to the conjugated pi-systems of the fullerene core or the sidewalls of single walled carbon nanotubes (SWNTs) is a very desirable task. In the last one and a half decade we have systematically investigated the basic principles of covalent fullerene- and SWNT chemistry and have synthesized and characterized hundreds of derivatives with very interesting physical-, biomedical and materials properties.[1,2] A selection of such new functional carbon-rich compounds including their hierarchical supramolecular organization will be presented.[3] A major key point for the synthesis of fullerene- and SWNT derivatives with tailor made properties is to achieve control over chemo- and regionselectivity of addition reactions. In this presentation we will also demonstrate both inherent selectivity principles of the carbon allotropes themselves, such as the preferred addition to metallic and small diameter SWNTs, as well as the development of chemical concepts for their highly selective functionalization, such as the tether controlled synthesis of hexakisadducts of C60 with an octahedral addition pattern.

- 1 A. Hirsch, M. Brettreich, Fullerenes, Chemistry and Reactions, Wiley-VCH, Weinheim, 2004.
- 2 a) A. Hirsch, Angew. Chem. Int. Ed. 2002, 41, 1853, b) O. Vostrowsky, A. Hirsch, Angew. Chem. 2004, 116, 2380-2383; Angew. Chem. Int. Ed. 2004, 43, 2326-2329.
- 3 a) R. Graupner et al., J. Am. Chem. Soc. 2006, 128, 6683-6689, b) J. Dannhaeuser et al., Angew. Chem. Int. Ed. 2006, 45, 3368-3372; c) U. Hartnagel et al., Angew. Int. Ed. 2007, 46 4293; O. Vostrowsky, A. Hirsch, Chem. Rev. 2007, 106, 5191.

11:30

Study of Nano-Carbons by Aberration Corrected Low Voltage Electron Microscopy

U. Kaiser¹ A. Chuvilin¹ D. Obergfell² S. Roth²

¹University of Ulm, Central Facility of Electron Microscopy, Electron Microscopy Group of Materials Science, Albert Einstein Allee 11, 89069 Ulm, Germany

²Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany.

Over the last few years the performance of transmission electron microscopes has undergone an enormous improvement with revolutionary advances in both spatial resolution and spectroscopic capability including its energy resolution. This has been made possible through the development of electron optical components for the correction of the intrinsic aberrations present in conventional electromagnetic round lenses. It is now possible to acquire atomic resolution structural data from a wide range of materials even imaging light elements such as carbon. This talk will provide a brief overview of the basics of this development and of the instrumental advances emphasizing the new insights that they can provide to several areas of materials science on the example of nano-carbons. We will report on direct observation of carbon atoms and dynamical processes in $(Dy@C_{82})@SWNT$ metallofullerene peapods.

Non-carbon materials, Fullerenes, DWNT

Wednesday, March 5

18:30

Catalysis Chemistry of the Confined Nano-Systems

Xinhe Bao^{1,2}

¹Dalian Institute of Chem. Phys., Chinese Academy of Sciences, Dalian

²State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, the Chinese Academy of Sciences, Dalian 116023, P. R. China

This talk will be focused on the application of nano-related science and technology in the fields of catalysis, with an emphasis on the electron properties of the confined systems and the synergetic confinement effects between the encapsulated metallic nanoparticle and carbon nanotubes. (1) The effect of electron quantum confinement on the catalytic activities of 2D ultra-thin metal films is explored by comparing the work function change and the initial reaction rate of atomically flat films of different thickness on silicon surfaces, using complementary microscopy and spectroscopy techniques. The obvious oscillations of the oxidation rate of lead films are observed, which are attributed to be a manifestation of the Fabry-Pérot interference modes of electron de Broglie waves (quantum well states) in the films. The modulation of the electron density of states near the Fermi level opens a new demission for tuning the catalytic performance of metal systems via size- and thickness-dependent quantum size effects, which will be illustrated through two examples. (2) Carbon nanotubes (CNTs) have well defined hollow interiors and exhibit unusual mechanical and thermal stability as well as electron conductivity. This opens intriguing possibilities to introduce other matter into the cavities, which may lead to nanocomposite materials with interesting properties or behaviour different from the bulk. In the present talk, two unique properties concerning the redox and catalysis of the CNT-encapsulated metals and metal oxides will be addressed. The autoreduction of the encapsulated Fe₂O₃ is significantly facilitated inside CNTs with respect to the outside nanoparticles, and it becomes more facile with decreasing CNT channel diameter as evidenced by temperature programmed reaction, in situ XRD and Raman spectroscopy. The oxidation of encapsulated metallic Fe nanoparticles on the other hand is retarded in comparison to that of the outside Fe particles as shown by in situ XRD and gravimetrical measurements with an online microbalance. A striking enhancement of the catalytic activity of Rh particles confined inside nanotubes for the conversion of CO and H2 to ethanol has been found. The overall formation rate of ethanol inside nanotubes exceeds that on the outside of the nanotubes by more than an order of magnitude, although the latter is much better accessible. We attribute these unique behaviours of transition metal nanoparticles inside CNTs to a particular electronic interaction of the encapsulates with the interior CNT surface.

References:

- 1. Xiulian Pan et al., Nature Materials, 6(2007)507-511
- 2. Wei Chen et al., J. Am. Chem. Soc., 129(2007)(23)7421-7426
- 3. Xucun Ma et al., P NATL ACAD SCI USA (PNAS), 104(2007)(22)9204-9208
- 4. Junning Sun et al., J. Am. Chem. Soc., 128 (49) (2006) 15756-15764

5. Wei Chen et al., J. Am. Chem. Soc., 128 (10) (2006) 3136-3137x

19:00

Modification of Carbon Nanotube Architectures for Alternative Energy Applications

Andrew Minett

Intelligent Polymer Research Institute, University of Wollongong, Wollongong, Australia

Due to their high surface area, eletro-chemical stability and versatility, carbon nanotube electrodes have been attracting great interest for use in alternative energy applications such as supercapacitors, Li-ion batteries and fuel cells. In this presentation, we describe the production and modification of flexible pre-formed carbon nanotube architectures with various entities such as conducting polymers or metal nanoparticles for use as superior electrode materials. Recently, we have reported on the direct use of various carbon nanotube assemblies as electrodes for Li-ion batteries, supercapacitors or catalyst supports. In one process, a flexible aCNT/PEDOT/PVDF membrane electrode is prepared via conventional CCVD. This electrode structure was assembled into a lithium-ion battery for testing, by stacking a porous polypropylene separator containing liquid electrolyte between the aCNT/PEDOT/PVDF electrode and a lithium-foil counter electrode. While this assembly showed a large irreversible first cycle capacity, a highly stable discharge capacity of 265 mAh/g is observed for the second to fiftieth cycle. In a second related approach, a novel carbon composite electrode shows vastly superior reversible capacities of over 600mAh/g, stable over 100 cycles. What is remarkable with this electrode system is that there is no large drop in capacity during charge cycles. To demonstrate the versatility of these carbon composite electrodes, the introduction of metal nanoparticles for catalysis or enhanced electrochemical properties allows the use of these electrodes as either the anode or cathode in fuel cell applications or as supercapacitors. Eight different metals have been deposited by a simple method with nanoparticle sizes as small as 4nm. Energy densities of 70Wh/kg and power densities up to 10kW/kg for these composite electrodes highlight promise for alternative energy applications.

19:30

Gallium Nitride Nanowires: Impurity and Disorder Effects on Thermal Conductivity

<u>Jack Fischer</u>¹ Csaba Guthy² Chang-Yong Nam³ Douglas Tham⁴

¹Materials Science and Engineering, Uinversity of Pennsylvania, Philadelphia, PA

²University of Alberta, Saskatchewan Canada

³Brookhaven National Laboratory, Upton NY USA

⁴California Institute of Technology, Pasadena CA USA

Gallium nitride is an important large-gap high mobility semiconductor for high power optoelectronic and fast-switching electronic applications, both of which require high thermal conductivity for heat dissipation. Limitations in bulk crystal growth and epitaxial film deposition motivate in part a growing interest in GaN nanowires, so it is important to understand and control thermal properties at the nanoscale.

In this study we measured the thermal conductivity of individual GaN NWs grown by thermal chemical vapor deposition (CVD) with diameters ranging from 97 to 181 nm, using the "suspended islands" method. We observed unexpectedly large reduction compared to the bulk, with room temperature values in the range 13-19 W/mK and weak diameter dependence. We also observe unusual $T^{1.8}$ power law dependence at low T. The Callaway model suggests only moderate reduction due to increased boundary scattering for small cross-sections. TEM analysis revealed the presence of stacking faults which limit the phonon mean free path. Furthermore, EELS measurements indicate high Si and O impurity concentrations estimated at 0.1-1 at% and 0.01-0.1 at%, respectively. Based on extensive numerical calculations we conclude that both the unexpectedly low thermal conductivity as well as the $T^{1.8}$ low-temperature dependence are caused by unusually large mass-difference scattering, primarily from Si impurities. Our analysis also suggests that the mass-difference scattering rates are significantly enhanced by the reduced phonon group velocity in nanoscale systems.

Supported by DOE Grant No. DE-FG02-98ER45701.

20:00

Mode-locked 177-fs soliton erbium-doped fiber laser based on a cellulose polymer film containing carbon single-wall nanotubes synthesized by the arc-discharge method

 $\underline{\rm Anton~Tausenev}^1$ Elena Obraztsova² Anatolii Lobach³ Petr G. Kryukov¹ Alexander Chernov⁴ Vitaly Konov² Eugeny Dianov¹

Non-linear optical properties of single-wall carbon nanotubes (SWNTs) is a basis for new optical media for ultrafast modulation for mode-locked fiber lasers. In this work we demonstrate a new mode-locked soliton erbium-doped fiber laser generating 177-fs pulses. The laser pumped by a 85-mW, 980-nm laser diode emits 7 mW at 1.56 um at a pulse repetition rate of 50 MHz. Passive mode-locking is achieved with the help of a saturable absorber made of a high-optical quality film based on cellulose derivatives with dispersed carbon single-wall nanotubes. The film is prepared by the original technique by using carbon nanotubes synthesized by the

¹Fiber Optics Research Center RAS, Moscow, Russia

²A.M. Prokhorov General Physics Institute, RAS, Moscow, Russia

³Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia

 $^{^4\}mathrm{Department}$ of Physics, M.V. Lomonosov Moscow State University, Moscow, Russia

Wednesday, March 5

Non-carbon materials, Fullerenes, DWNT $\,$

arc-discharge method.

Non-carbon materials, Fullerenes, DWNT

Wednesday, March 5

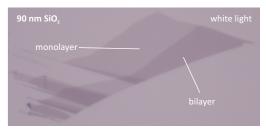


Providing graphene flakes and devices to industry and academia

Graphene on Si|SiO,

- We offer single, double, triple and >3 layer graphene flakes on 300 nm and 90 nm SiO₂.
- 90 nm SiO₂ is a new substrate that offers higher graphene contrast than the traditional 300 nm.
- Flakes are prepared from natural graphite using micromechanical cleavage.





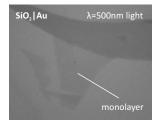
Flake sizes	Typically < 600 μm^2 ; largest monolayer found to date: 7000 μm^2
Pricing guide	≈ € 0.60 per μ m² area, with reductions if the flake is difficult to use for lithography, e.g. close to wafer's edge or surrounded by thick graphite flakes
Applications	transistors, spintronics, gas sensors, metrology, Raman spectroscopy, AFM, STM, etc.
Wafer sizes	min: 5 mm × 5 mm max: 76 mm diameter circle

Graphene on Si|SiO₂|Au

- We can isolate graphene flakes on gold using optical microscopy.
- A thin layer of gold is deposited onto an oxidised silicon wafer before preparing flakes.
- The gold layer is continuous and electrically conductive, but thin enough to maintain the optical interference effect that makes graphene visible.
- Narrow band-pass filters can be used to enhance the contrast.

Flake sizes	Typically < 400 μm²; largest monolayer found to date: 1000 μm²
Pricing guide	≈ € 3 per µm² area
Applications	STM, Raman spectroscopy
Wafer sizes	min: 5 mm × 5 mm; max: 25 mm × 25 mm





Visit GrapheneIndustries.com for more details and to see our current stock. If you have any questions, please do not hesitate to contact Tim Booth: tim@grapheneindustries.com

 ${\it Graphene\ Industries\ Ltd,\ 32\ Holden\ Avenue,\ Whalley\ Range,\ Manchester,\ M16\ 8TA,\ UK}$

Growth 8:30 - 9:30H. Kataura, JP Optical Properties of Metallic and Semiconducting Single-Wall Carbon Nanotubes 9:30 - 10:00J. Robertson, UK Carbon nanotubes as IC Interconnects 10:00 - 10:30 Coffee break 10:30 - 11:00 K. Hata, JP Super Growth: Working to Supply the World with Catalyst- $Free\ SWNTs$ 11:00 - 11:30 K. Suenaga, JP Imaging the carbon networks in carbon nanostructures 11:30 - 12:00 M. Terrones, MX The Importance of Defects in Carbon Nanotubes: How to Identify them using Different Techniques 12:00 - 17:00Mini Workshops 17:00 - 18:30Dinner 18:30 - 19:00 M. Hersam, US Preparation, characterization, and applications of monodisperse single-walled carbon nanotubes 19:00 - 19:30 S. Maruyama, JP Cross-polarized optical excitation of single-walled carbon nanotubes19:30 - 20:00M. Strano, UK Optical modulation of single walled carbon nanotubes for

chemical and biological detection

20:00 - 21:00 Poster Session - THU

Thursday, March 6

8:30

Optical Properties of Metallic and Semiconducting Single-Wall Carbon Nanotubes

<u>Hiromichi Kataura</u>¹ Yasumitsu Miyata² Kazuhiro Yanagi¹ Yutaka Maniwa² ¹Nanotechnology Research Institute, AIST, Tsukuba, Japan, and JST-CREST ²Department of Physics, Tokyo Metropolitan University, Tokyo, Japan, and JST-CREST

Recently, Arnold et al. have reported a new method to sort SWCNTs by their electronic types using a density gradient ultracentrifugation. [1] We have improved their method and successfully separated metallic and semiconducting SWCNTs in mass quantity with 99% purity. [2] We have measured electronic and optical properties of them with various diameters.

It was revealed that the metallic SWCNTs show bright colors, cyan, magenta, and yellow, depending on their mean diameter. [2] These colors are not strange because the metallic SWCNT has only one absorption band due to van Hove singularities in the visible range. The colorful SWCNTs could be used as highly durable full color conductive inks. Interestingly, conductivity of the metallic SWCNT thin film exhibited an extreme stability against a chemical carrier doping because of the constant electronic density of states near the Fermi level in the metallic SWCNT. [3] Resonance Raman spectra also showed very interesting results. It is well known that the frequency of D and G prime peak is depending on the excitation laser wavelength. This can be understood by the double resonance model which is concerning with the electronic band structure and the phonon dispersion. [4] It was found that the D and G prime peak frequency and their derivatives to the excitation energy of the metallic SWCNTs are different from that of the semiconducting ones. This result suggests an intrinsic difference in the physical properties of them.

- 1 M.S.Arnold et al., Nat. Nanotechnol. 1 (2006) 60.
- 2 Yanagi et al., submitted.
- 3 Y. Miyata et al. J. Phys. Chem. C (2008), accepted.
- 4 C. Thomsen and S. Reich, Phys. Rev. Lett. 85 (2000) 5214.

9:30

Carbon nanotubes as IC Interconnects

John Robertson

Engineering Dept, Cambridge University, Cambridge, UK

Carbon nanotubes have by far the highest current carrying capacity of any solid (1E9 A/cm2) and are generally proposed for interconnects in future integrated circuits. However, this application is not as secure as it may seem. The interconnects

must not only carry a high current but also have a lower resistance than the equivalent Cu version, bearing in mind that 1D conductors have an effective series quantum resistance. Secondly, for SWNTs, the net resistance depends on nanotube density, which is not so high. In practice this means that the obvious application of vertical interconnects (Vias) is less advantageous than the more difficult horizontal interconnects. Finally, chirality selection is an issue as we must selectively grow metallic nanotubes, preferably at low temperature. Developments in the growth or deposition, characterisation and modelling on CNT interconnects are described.

10:30

Super Growth: Working to Supply the World with Catalyst-Free SWNTs Kenii Hata

National Institute of Advanced Industrial Science and Technology, Tsukuba

In addition to scientific innovation, the development of carbon nanotube (CNT) technology (and consequently a CNT-based industry) is reliant upon the availability of CNTs. In particular, the extremely high commercial cost of single-walled carbon nanotubes (SWNTs), stemming from the lack of efficient and cleanflynthesis, represents a significant obstacle to wide-range industrial and scientific. However to realize this, not only is an efficient and pure process necessary, low-cost scalability plays a critical role which Super-growth CVD [1] has emerged as an emerging technology to overcome this barrier. This presentation will provide an overview of our recent development of carbon nanotube synthesis and their applications based on the SSuper GrowthCVD in particular our efforts for industrial-scale mass production. After providing a brief introduction to the Super-Growth concept, I will outline our major challenges and recent progress toward the realization of industrial-scale mass production of high-purity, long, and aligned SWNTs to establish a carbon nanotube-based industry.

11:00

Imaging the carbon networks in carbon nanostructures

Kazu SUENAGA AIST, Tsukuba

Physical and chemical properties of carbon nanotubes can be drastically altered by its atomic defects and chirality. Imaging of the carbon networks is therefore of prime importance to characterize the carbon nanotubes and has been recently made possible by pushing the HR-TEM to the extreme of its possibilities. In this presentation some examples for the atomic-level characterization of carbon nanotubes and their derivatives by means of the HR-TEM will be demonstrated. The topics involves the stability and mobility of atomic defects in carbon nanotube (1,2) and the embedded/attached molecules within nanotubes (3,4,5).

The presented work is partially supported by CREST-JST, ERATO-JST, NEDO,

KAKENHI and JSPS.

- 1 K. Suenaga et al., Nature Nanotech. 2 (2007) 358
- 2 C.-H. Jin et al., Nature Nanotech. 3 (2008) 17
- 3 Z. Liu et al., J. Am. Chem. Soc., 129 (2007) 6666
- 4 Z. Liu et al., Nature Nanotech. 2 (2007) 422
- 5 Y. Sato et al., Nano Lett., 7 (2007) 3004

11:30

The Importance of Defects in Carbon Nanotubes: How to Identify them using Different Techniques

Mauricio Terrones

Advanced Materials Department, IPICYT, San Luis Potosi

In this talk, defects within carbon nanotubes will be categorized in 4 different groups: (1) Structural defects, related to imperfections that significantly distort the curvature of the hexagonal carbon honeycomb structure; these defects are usually caused by the presence of non-hexagonal rings (e.g. pentagons, heptagons, or octagons; (2) Topological defects, occurring on the nanotube surface, which do not result in large curvature distortions of the tubule. In particular, these defects could be 5-7 pairs embedded in the hexagonal network or Stone-Wales (SW-type) defects that could be created by rotating a carbon bond within 4 neighboring hexagons, thus resulting in the transformation of 2 pentagons and 2 heptagons; (3) Doping-induced defects, arising from substitutional non-carbon atoms embedded (or incorporated) into the tubular lattice, and (4) Non-sp2 carbon defects or edge-sites caused the presence of highly reactive carbons such as dangling bonds, carbon chains, interstitials (free atoms trapped between SWNTs or between graphene sheets), edges (open nanotubes), add-atoms and vacancies.

From the theoretical standpoint, the structural stability and electronic properties of nanotubes containing hexagons, pentagons and heptagons will also be discussed in detail. These structures, now termed Haeckelites, are predicted to be metallic and exhibit enhanced electronic conductances when compared to standard pure carbon nanotubes. High resolution transmission electron microscopy (HRTEM) studies and theoretical calculations reveal that these type of structures are likely to be synthesized.

This presentation will review recent work related to different techniques used to identify defects using HRTEM, scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), Raman spectroscopy (RS), atomic force microscopy (AFM), thermogravimetric analyses (TGA), electron and thermal transport measurements, etc. It is important to mention that most of the time the presence of

Thursday, March 6

Growth

defects and their identification has been overlooked by numerous scientists. However these play a key role in the nanotubes physico-chemical properties. There are numerous challenges that will be discussed in this presentation: How do we identify defects efficiently? Could we distinguish among various defects? Would it be possible to establish a protocol able to quantify and control the amount of these defects? How many defects are necessary to fabricate robust polymer composites or nanotube junctions? Could we observe ferromagnetism in defective nanocarbons?, etc.

Growth Thursday, March 6

18:30

Preparation, characterization, and applications of monodisperse single-walled carbon nanotubes

Mark C. Hersam

Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208-3108 USA

Large-scale production of monodisperse single-walled carbon nanotubes (SWNTs) has the potential to enable and/or improve many applications for SWNTs such as thin film transistors, transparent conductors, optical amplifiers, and biosensors. Recently, we have developed a scalable and flexible technique for sorting SWNTs by their physical and electronic structure using density gradient ultracentrifugation (DGU) in aqueous solution [1-3]. For sorting by physical structure, DGU exploits inherent differences in buoyant density as a function of SWNT diameter. Alternatively, for sorting by electronic structure, DGU takes advantage of subtle differences in buoyant density that result from differential adsorption of co-surfactant mixtures to metal versus semiconducting SWNTs. This talk will delineate recent developments in DGU including efforts to improve purity, yield, and throughput of monodisperse SWNTs. In addition, this talk will explore the improvements that monodisperse SWNTs enable in both fundamental experiments and applied technologies. For example, SWNTs sorted by DGU enable unambiguous interpretation of SWNT exciton dynamics in ensemble pump-probe spectroscopy measurements [4]. From a technology perspective, chirality-resolved SWNTs allow the optical and electrical properties of semi-transparent, conductive films to be independently tuned. Specifically, the ability to sort metallic SWNTs by diameter enables the formation of conductive films with tunable optical adsorption throughout the visible and infrared portion of the electromagnetic spectrum. The properties and potential applications of this semi-transparent, conductive SWNT stained glass will be discussed. This talk will conclude with the prospects of DGU for sorting other nanomaterials by their physical and electronic structure.

- 1 M. S. Arnold, et al., Enrichment of single-walled carbon nanotubes by diameter in density gradients, Nano Letters, 5, 713 (2005).
- 2 M. S. Arnold, et al., Sorting carbon nanotubes by electronic structure via density differentiation, Nature Nanotechnology, 1, 60 (2006).
- 3 A. A. Green and M. C. Hersam, Ultracentrifugation of single-walled carbon nanotubes, Materials Today, 10, 59 (2007).
- 4 Z. Zhu, et al., Pump-probe spectroscopy of exciton dynamics in (6,5) carbon nanotubes, J. Phys. Chem. C, 111, 3831 (2007).

19:00

Cross-polarized optical excitation of single-walled carbon nanotubes

Shigeo Maruyama

Department of Mechanical Engineering, The University of Tokyo, Tokyo

Because of the depolarization effect, or so-called antenna effect, cross-polarized optical absorption of single-walled carbon nanotubes (SWNTs) is believed to be quite weak. However, in photoluminescence (PL) excitation spectra of micelle wrapped SWNTs, clearly identified PL peaks due to cross-polarized excitation gives an important measure of optical transition energy of E12 or E21 [1]. The cross-polarized absorption must be dominant in the absorption of vertically aligned film of SWNTs [2] when excited from the top of a film. In our previous study of polarized UV/Vis absorption, pi-plasmon absorption at 5.25 eV was revealed in contrast to 4.5 eV for parallel excitation [3]. The consistent physical view of electron energy loss spectroscopy (EELS) is now being explored [4] with the understanding that the bundle side of such a vertically aligned SWNT film is as small as 5-8 nanotubes [5]. Detailed polarized Raman study is performed to further study the anisotropic optical properties of SWNTs.

- 1 Y. Miyauchi, M. Oba, S. Maruyama, Phys. Rev. B 74 (2006) 205440.
- 2 Y. Murakami et al., S. Chiashi, Y. Miyauchi, M. Hu, M. Ogura, T. Okubo, S. Maruyama, Chem. Phys. Lett. 385 (2004) 298.
- 3 Y. Murakami, E. Einarsson, T. Edamura, S. Maruyama, Phys. Rev. Lett., 94 (2005) 087402.
- 4 C. Kramberger, R. Hambach, C. Giorgetti, M. H. RAummeli, M. Knupfer, J. Fink, B. BAuchner, L. Reining, E. Einarsson, S. Maruyama, F. Sottile, K. Hannewald, V. Olevano, A. Marinopoulos, T. Pichler, submitted to Phys. Rev. Lett.
- 5 E. Einarsson, H. Shiozawa, C. Kramberger, M. H. Ruemmeli, A. Grüneis, T. Pichler, S. Maruyama, J. Phys. Chem. C, 111 (2007) 17861.

19:30

Optical modulation of single walled carbon nanotubes for chemical and biological detection

Michael S Strano

Department of Chemical Engineering, MIT, Cambridge

Nanoscale sensing elements offer promise for single molecule analyte detection in physically or biologically constrained environments. Molecular adsorption can be amplified via modulation of sharp singularities in the electronic density of states

that arise from 1D quantum confinement. Single-walled carbon nanotubes (SW-NT), as optical sensors^{1,2}, offer unique advantages such as photostable near-infrared (n-IR) emission for prolonged detection through biological media, single-molecule sensitivity and, nearly orthogonal optical modes³ for signal transduction that can be used to identify distinct classes of analytes. This presentation will describe our efforts to understand chemically induced optical modulation of carbon nanostructures and their development in various sensor applications.

- 1 DA Heller, et al.. Science 311 (2006) 508-511.
- 2 PW Barone, et. al. Nature Materials 4 (2005) 86-92.
- 3 Choi, J. H. and Strano, M. S. Applied Physics Letters. 90 (2007) 22314.

Growth Thursday, March 6

Combined STM/STS, TEM/EELS and optical absorption investigation of CxNy-SWNTs

 $\underline{H.\ Lin}^1$ J. Lagoute 2 C. Chacon 2 V. Repain 2 L. Bresson 1 S. Enouz 1 J-S. Lauret 3 S. Rousset 2 A. Loiseau 1

¹LEM UMR 104, ONERA-CNRS, BP 72, 92322 Chatillon, France

 $^2\mathrm{MPQ},\,\mathrm{UMR}$ 7162 Universite Paris Diderot, CNRS, Case 7021, 72205 Paris Cedex 05, France

³LPQM, ENS Cachan, France

Carbon nanotubes are tubular structures with unique electronic properties, which can further be modified by adding hetero-atoms such as boron or nitrogen into the carbon network. By combining STM/STS and TEM/EELS techniques, the objectives of this study are first to identify the hetero-atoms present in the carbon network and then to understand their role on the electronic structures. Whereas TEM/EELS provides useful information on the morphology of the tubes and their concentration in hetero-atoms, STM and STS have been shown to be powerful techniques for investigating the relationship between the atomic and electronic structures since atomic resolution images of nanotubes can be achieved together with local spectroscopy. To this aim, $C_x N_y$ -SWNTs have been synthesized by vaporizing by a CO_2 continuous laser a C:Ni\Y target under a nitrogen atmosphere. According to TEM observations, the tubes are mostly single-walled and display a very similar morphology to that obtained under a helium atmosphere. EELS analysis indicate a nitrogen concentration lower than 1at.%. STM observations of both pure C-SWNTs and C_xN_y -SWNTs have been then performed. For both kinds of tubes, atomic resolution images have been obtained by STM as well as STS spectra, from which electronic density of states have been extracted and compared to optical absorption spectra. Comparison of the results for both kinds of tubes and discussion will be given in the poster.

2

NOVEL APPROACHES TO PURIFICATION OF SINGLE-WALL BORON NITRI-DE NANOTUBES

<u>Anatoly Lobach</u>¹ Natalia Spitsina¹ Elena Obraztsova² Natalia Arutyunyan² Annick Loiseau³ Aude Maguer³ Lionel Bresson³

¹Institute of Problems of Chemical Physics Russian Academy of Sciences, Chernogolovka, Russia

²A.M. Prokhorov General Physics Institute RAS, 38 Vavilov Street, 119991 Moscow, Russia

³LEM, ONERA-CNRS, BP72 92322 Chatillon Cedex, France

A raw materials of single-walled boron nitride nanotubes (SWBNNT) contains several components in addition to nanotubes: boric acid, boron oxide, and nano-

particles of h-BN [1]. The method for purification of the SWBNNT raw materials based on the difference in solubility of the components of the material and their density was developed [2]. Novel approaches developed for the purification consists of two main steps: 1, removal of boric acid and boron oxide; 2, separation of the residual material by density using centrifugation of its suspension in a methanol. The SWBNNT raw material and its components obtained after the purification process were characterized by IR, Raman spectroscopy and TEM. The SWBNNT material obtained after purification is highly dispersed in polar solvents (methanol, ethanol) and in an aqueous solution of the carboxymethylcellulose (CMC) polymer, indicating that the nanotube surface contains polar groups. The films of the CMC polymer containing the SWBNNT material of optical quality were produced. The work is supported by INTAS-05-1000008-7871.

- 1 A. Loiseau et al., Phys. Rev. Lett. 76, 4737 (1996).
- 2 A. Maguer et al., J. Nanosci. Nanotechnol. 7, 3524 (2007).

3 Optically Excited Carbon Nanotube as a Tonks–Girardeau Gas

Richard M. Russo¹ <u>David E. Luzzi</u>² Eugene J. Mele³

¹Dept. of Materials Science, University of Pennsylvania, Philadelphia, PA, 19104, US

²College of Engineering, Northeastern University, Boston, MA, 02115, US ³Dept. of Physics, University of Pennsylvania, Philadelphia, PA, 19104, US

The fundamental optical excitations of carbon nanotubes are excitons, charge neutral bound states of excited electron hole pairs. Excitation at high intensity produces a dense one dimensional excitonic liquid, a nonequilibrium state controlled by interexciton interactions and their Bose statistics. Previous work has focused on the time evolution of the many exciton state to its dilute regime. In this paper, we use the history dependence of transient pump-probe absorption spectra from isolated carbon nanotubes to probe interexciton correlations and dynamics at high excitation density. Interestingly we find a dependence of these spectra on the exciting fluence and the pump-probe time delay well described by the interparticle correlations of the Tonks-Girardeau gas where hard wall repulsive interactions between excitons govern their nearest neighbour correlations and chemical potential. Fits of the model to experiment provide a direct measurement of the exciton diffusion constant.

Carbon nanotubes - Vanadium oxides composite: Synthesis and Applications

Arnaud Magrez¹ Barbara Korbely² Laszlo Forró¹

¹Ecole Polytechnique Federale de Lausanne, Switzerland

²Ecole Polytechnique Federale de Lausanne, Switzerland and University of Szeged, Hungary

Vanadium oxides VOx like V_2O_5 , VO_2 or V_2O_3 are promising materials for numerous applications like power sources and thermochromic based devices. Composites with carbon nanotubes are of particular interests to enhance both the electronic and thermal conductivity of these functional materials. We have developed a preparation process of the composite by an in situ growth of carbon nanotubes at low temperature on nanostructured VOx using the equimolar acetylene- CO_2 reaction [1]. The carbon nanotubes content can be easily controlled as well as the oxidation state of the vanadium cations by the growth conditions of the CNTs and a post heat treatment of the composite under air. Based on these composites, lithium ion batteries and thermochromic windows have been built and characterised.

 A. Magrez, J.W. Seo, V.L. Kuznetsov and L. Forró, Angewandte Chemie Int. Ed. 2007, 46, 441

5

Formation of curved graphite sheets and eclipsed sp3 bonds in nanographite followed by Raman spectroscopy

<u>Tatiana L. Makarova</u>¹ Mauro Ricco² Daniele Pontiroli² Marcello Mazzani² Matteo Belli² Angelo Goffredi²

¹Physics, Umea University, Umea

²CNISM and Dipartimento di Fisica, Universita di Parma, Italy.

The formation of curved graphite-like structures during annealing of diamonds is a well studied phenomenon. Here we present the observation of an opposite process, the formation of the sp3-bonded carbons and onion carbon shells during the room-temperature hydrogenation of ball-milled nanographite. Three distinct peaks are observed in the low wavenumber region, at about 1100, 860, and 450 cm-1, whereas the G peak is softened. The origin of these peaks is discussed in terms of curvature of the graphene planes. Strong T-band at 1100 cm-1, which is quite rarely detected in visible Raman scattering experiments, indicates the presence of sp2/sp3 alternating hybridization. This band has recently been attributed to the presence of eclipsed bonds, forming fused pentagonal rings. The strain of graphene planes due to curvature caused by introducing pentagons can account for the downward shift of the G peak.

Electronic and phonon properties of monolayer and bilayer graphene probed by resonance Raman scattering

<u>Leandro M Malard</u>¹ D. L. Mafra¹ D. C. Elias¹ J. C. Brant¹ F. Plentz¹ E. S. Alves¹ M. A. Pimenta¹ J. Nilsson² A. H. Castro Neto² G. Samsonidze³

 1 Departamento de Física, Av. Antônio Carlos, 6627, Belo Horizonte, 30123-970, MG, Brazil

 $^2\mathrm{Department}$ of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA

³Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA

Monolayer graphene has attracted a great amount of interest due to its linear dispersion around the K point in first Brillouin zone, giving an insight to new physics and device applications. On the other hand, bilayer graphene is a zero gap semiconductor with a parabolic dispersion near the K point, providing interesting new properties as a tunable gap system by applying an electric field. In this work, we show that, by measuring second order Raman bands associated with a double resonance Raman process as function of laser energy, we can probe both the electronic and phonon dispersion relations for mono and bilayer graphene. For monolayer graphene, we have been able to probe the in-plane transversal optic (iTO) and longitudinal acoustic (LA) modes by measuring the dispersion of the G' and G* (around 2450 cm⁻¹) bands, and the results are compared with phonon calculations in the literature [1]. For bilayer graphene, the measurement with different laser lines of the four peaks that comprise G' band provides experimental values of the Slonczewski-Weiss-McClure band structure parameters [2]. These results show that resonance Raman spectroscopy is a useful tool to probe phonons and electrons in these novel materials.

- 1 D. L. Mafra et al., Phys. Rev. B **76**, 233407 (2007).
- 2 L. M. Malard et al., Phys. Rev. B **76**, 201401(R) (2007).

7

Coulomb effects in carbon nanotubes

 $\underline{\rm Ermin\ Mali\acute{c}^1}$ Matthias Hirtschulz^1 Frank Milde
¹ Marten Richter^1 Janina Maultzsch^2 Stephanie Reich³ Andreas Knorr^1

We present a microscopic calculation of the excitonic absorption coefficient for single-walled carbon nanotubes. Our approach combines the density matrix formalism including the Coulomb and electron-light interaction with the tight-binding

¹Theoretische Physik, Technische Universität Berlin, Berlin

²Festkörperphysik, Technische Universität Berlin, Berlin

³Fachbereich Physik, Freie Universität Berlin, Berlin

approximation. We go beyond the two-band picture taking into account all intraand intersubband contributions and study the behavior of the Coulomb matrix elements for all relevant scattering processes. Our approach allows the investigation of excitons in single-walled carbon nanotubes of arbitrary chiral index over a wide range of energy. Both the energy renormalization due to the electron-electron coupling and the formation of excitons due to the electron-hole coupling are discussed. We show the diameter and chirality dependence of excitonic effects presenting Kataura plots for the first, second and third optical transition. The excitonic character of optical excitations in carbon nanotubes is shown not to be restricted to the first two transitions. Finally, we discuss the dark-bright splitting of excitonic states being a consequence of the K-K Coulomb intervalley mixing.

8 Reversible Local Metal-Insulator Transition in Metallic Single-Walled Carbon Nanotubes

<u>Christoph W Marquardt</u>¹ Aravind Vijayaraghavan¹ Simone Dehm¹ Frank Hennrich¹ Ralph Krupke¹

 $^1{\rm Forschungszentrum}$ Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany

Metal-insulator transition in metallic single-walled carbon nanotubes (mSWNT) induced by electron irradiation has been recently reported [1,2]. In these previous studies the whole device has been irradiated including the contact regions. To study this effect in more detail, we restrict in this work electron irradiation to a narrow nanotube segment distant from the contacts. Devices were manufactured by dielectrophoretic nanotube deposition [3]. Prior to electron irradiation we conditioned the device by a novel procedure to obtain the lowest contact resistance possible for nanotubes with approx. 1nm diameter [4]. After this conditioning the structures show linear (metallic) IVs and a current saturation in the high bias regime typical for low contact resistance devices [5]. Afterwards we performed multiple SEM linescans across the mSWNT. These scans cause a local metal-insulator transition in the mSWNT [1,2] which lead to an increasing nonlinearity in the IV as well as a decrease of the low-bias-conductivity. Interestingly this local metal-insulator transition proves to be reversible, since the low-bias conductance observed before the scanning can be reestablished by a further voltage ramping procedure.

- 1 A. Vijayaraghavan, Nano Letters 5 (2005)
- 2 K. Kanzaki, Journal Of Applied Physics 101 (2007)
- 3 R. Krupke, Nano Letters 3 (2003)
- 4 W. Kim, Applied Physics Letters 87 (2005)
- 5 Z. Yao, Physical Review Letters 84 (2000)

9 CVD growth of carbon nanotubes: study of the catalyst-substrate interaction

<u>Cecilia Mattevi</u>¹ John Robertson² Stephan Hofmann² Christoph Tobias Wirth² Mirco Cantoro³ Cinzia Cepek⁴ Carla Castellarin-Cudia⁵ Andrea Goldoni⁵

¹AREA Science Park, Padriciano 99, I-34012 Trieste, Italy

²Department of Engineering, University of Cambridge, Cambridge CB3 0FA, UK ³IMEC, AMPS/NANO, Kapeldreef 75, 3001 Leuven, Belgium

⁴Laboratorio Nazionale TASC-CNR-INFM, ss 14, km 163.5, I-34012 Trieste, Italy ⁵Surface Science Division, Sincrotrone Trieste SCpA, ss 14, km 163.5, I-34012 Trieste, Italy

To achieve the desired degree of carbon nanotube s (CNT) crystallinity and chirality via catalytic assisted chemical vapour deposition (CVD), it is important to identify the key parameters driving the CNTs growth. Amongst them, the catalyst supports is an important parameter which affect the rate, yield and growth direction of CNT obtained via CVD [1-3]. However till date very little efforts have been made to understand, how the substrate-catalyst interaction determines the chemical state and the morphology of the catalyst nanoparticles before and during the growth [3]. In this respect, the importance of the catalyst nanoparticle-substrate interaction in the CNT growth via surface-bound CVD has been verified by performing a systematic study of CNT growth in different experimental apparatus. We used different substrates (Al_2O_3 and SiO_2), Fe as catalyst, and C_2H_2 as carbon source. The CVD growths have been performed in significantly different conditions: at very low growth pressure of C_2H_2 (8 × 10⁻⁶ mbar) in an ultra high vacuum chamber (UHV), and at high growth pressure (atmospheric pressure, in a conventional furnace). We underline that the same CVD process and catalyst pretreatments were performed in each experimental apparatus on both, Al_2O_3 and SiO_2 substrates. In agreement with literature [1,2], our experimental data show that the CNTs growth yield is significantly enhanced on Al_2O_3 , and this behavior was observed in all experimental apparatus we used. In particular in the furnace we were able to obtain vertical CNT arrays (forests), which could only be grown on Al_2O_3 , whereas the same process performed on SiO_2 , gave only lateral growth with lower CNTs density. In the UHV apparatus we were able to monitor in situ by means of X-ray photoemission spectroscopy (XPS) all the steps of the CVD route, avoiding any contamination due to air. Our XPS data indicate that Fe interacts with the oxygen of the surface layer of Al_2O_3 , whereas in case of SiO_2 this interaction doesn t take place. As a result of this interaction of Al_2O_3 , the mobility of Fe particles is reduced, preventing their coalescence in to large islands during annealing. The narrower size distribution and the limited mobility of the particles on Al_2O_3 as compared to SiO_2 , lead to a more uniform growth rate of CNTs, hence allowing their vertically aligned growth. In addition our XPS data also shows that the growth of any form of tubular carbon is inhibited when the Fe catalyst films is completely oxidized: the massive CNTs growth were observed on Al_2O_3 only when the catalyst films presents the coexistence of both, metallic and oxidized Fe.

- 1 K. Hata, D. N. Futaba, K. Mizuno, T. Namai, M. Yumura, and S.Iijima, Science 306, (2004), 1362.
- 2 S.Noda, K. Hasegawa, H.Sugime, K.Kakehi, Z. Zhang, S.Maruyama, and Y. Yamaguchi, Jpn. J. Appl. Phys. 46, (2007), 399.
- 3 T. de los Arcos, M.G. Garnier, J.W. Seo, P. Oelhafen, V. Thommen, D. Mathys, J. Phys. Chem. B 108, (2004), 7728.

10

¹H NMR spin-lattice relaxation in C₆₀-cubane

M. Bokor¹ <u>P. Matus</u>¹ P. Banki¹ K. Tompa¹ G. Kriza¹ E. Kovats¹ S. Pekker¹ G. Benyei² I. Jalsovszky²

¹Research Institute for Solid State Physics and Optics, Budapest, Hungary

We have investigated the rotor-stator molecular crystal fullerene-cubane ($C_{60} \cdot C_8 H_8$) by $^1 H$ NMR spectroscopy in the temperature range of 100 K to 380 K. The $^1 H$ line is broad and exhibits fine structure characteristic of a multispin spectrum, indicating the absence of angular reorientations of the cubane molecule. The spin-lattice relaxation rate displays a broad maximum at a magnetic field dependent temperature. The field dependence is much weaker than expected for field fluctuations arising from molecular reorientations. Possible underlying mechanisms are discussed.

11

Lattice Dynamics of Graphene and Graphite

Karl H. Michel¹ B. Verberck²

¹Department of Physics, University of Antwerp, Antwerp (B)

Starting from a harmonic lattice dynamical model, we present analytical and numerical results on the phonon dispersion relations and the elastic properties of graphite, single layer graphene and multilayer graphene systems. The lattice dynamical model is based on an atomic force constants model for the covalent atom-atom bonds within a graphene layer and an atom-atom Lennard-Jones potential for the weak van der Waals interactions between layers. The inter-plane force constants up to fifth-nearest neighbors are those determined from recent x-ray scattering experiments [1]. Using Born s long-wavelength method we determined the elastic constants (i.e. tension coefficients) for in-plane deformations of graphene as well as the elastic constants of graphite. We derive the elastic energies for stretching and for bending of graphene. Within the present force constants model for out-of-plane displacements, the bending rigidity κ_b of graphene has the value of ≈ 1 eV. This

²Department of Organic Chemistry, Eotvos Lorand University, Budapest, Hungary

²Institut fuer Festkoerperforschung, Juelich Forschungszentrum, Juelich (D)

large value is in good agreement with the result of atomistic Monte Carlo simulations [2] based on a many-body carbon bond-order potential. The value of κ_b leads to a macroscopically large persistence length ξ_p and favors the planarity of graphene.

- 1 M. Mohr, J. Maultzsch, E. Dobardzic, S. Reich, I. Milosevic, M. Damnjanovic, A. Bosak, M. Krisch, and C. Thomsen, Phys. Rev. B 76, 035439 (2007).
- 2 A. Fasolino, J.H. Los, and M.I. Katsnelson, Nature Mater. 6, 858 (2007).

12

Influence of the catalyst preparation on the final length of carbon nanotubes cut by grinding

Marijana Mionic¹ Arnaud Magrez¹ Laszlo Forró¹

CNTs grown by Catalytic Chemical Vapour Deposition (CCVD), can be up to tens of microns long. This is not suitable in particular to produce composite with polymer for microfluidics or NEMS applications. We have developed a method based on grinding to cut the carbon nanotubes down to 200nm length [1]. It is straightforward that the efficiency of the cutting process by grinding depends strongly on the diameter of the CNTs [2]. Indeed, the final CNTs length distribution will depend on the diameter distribution of the CNTs before grinding. It is known that the diameter of CNTs grown by CCVD is controlled by the size of the Fe₂Co metallic nanoparticles supported by CaCO₃. We have developed methods to produce the catalyst in order to control the CNTs diameter distribution [3]. The effect on the CNTs diameter distribution of the support particle size, precipitation method of Fe₂Co precursors on the support and the drying process of the catalyst will be presented.

- 1 M. Mionic, A. Magrez and L. Forró, to be submitted
- 2 N. Pierard, A. Fonseca, Z. Konya, I. Willems, G. Van Tendeloo, J. B. Nagy, Chem. Phys. Let. 2001, 335, 1.
- 3 M. Mionic, A. Magrez and L. Forró, to be submitted

Ecole Polytechnique Federale de Lausanne, Switzerland

Environmental effect on the cross-polarized optical transitions of singlewalled carbon nanotubes

Yuhei Miyauchi¹ Shigeo Maruyama¹

¹Dept. of Mech. Eng., The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Optical transition energies of single-walled carbon nanotubes (SWNTs) by the incident light polarized parallel to the nanotube axis such as E11 and E22 are known to be strongly affected by the change of environment around SWNTs [1, 2], which is called environmental effect. On the other hand, there is no report about the environmental effect for the cross-polarized excitations [3] to the nanotube axis. In this study, we have investigated the environmental effect on the tross-polarized excitations such as E12 and E21.

In our previous study [3], we found that some PL peaks for cross-polarized excitation to the nanotube axis can be clearly observed in the polarized PLE spectra of micelle-suspended SWNTs with relatively small diameters less than 1 nm. Recently, Lefebvre and Finnie [4] measured cross-polarized excitation energies of SWNTs in air with larger diameters more than 1nm. Here we have investigated the cross-polarized excitation energies of various (n, m) SWNTs with diameters more than 1 nm in a surfactant solution by polarized PLE spectroscopy. The observed excitation energies of micelle-suspended SWNTs for the cross-polarized condition are considerably red-shifted from those of SWNTs in air and the amount of the energy shift for cross-polarized excitations tended to be larger than those for parallel excitations. This result implies strong depolarization effect for cross-polarized excitations.

- 1 Y. Ohno, S. Iwasaki, Y. Murakami, S. Kishimoto, S. Maruyama, and T. Mizutani, submitted, (arXiv:0704.1018v1 [cond-mat.mtrl-sci])
- 2 Y. Miyauchi, R. Saito, K. Sato, Y. Ohno, S. Iwasaki, T. Mizutani, J. Jiang, S. Maruyama, Chem. Phys. Lett., 442, 394 (2007).
- 3 Y. Miyauchi, M. Oba, S. Maruyama, Phys. Rev. B 74, 205440 (2006).
- 4 J. Lefebvre, P. Finnie, Phys. Rev. Lett. 98, 167406 (2007).

First principles calculations of CdSe nanowires

Marcel Mohr¹ Christian Thomsen¹

¹TU Berlin, Berlin

We present first principles calculations of CdSe nanowires with diameters of up to 25 Å. Their atomic structure as well as electronic and vibrational properties are investigated. We verify the strong band gap dependence on nanowire diameter. In addition, passivating the surface dangling bonds increases the band gap. The evolution of phonon frequencies with decreasing diameter is analyzed. We find strongly size-dependent and nearly constant modes. We predict a low-frequency, diameter-dependent radial breathing mode (RBM) in CdSe nanowires

15

Diameter dependence of addition reactions to Carbon Nanotubes

 $\underline{\text{Matthias Müller}}^1$ Janina Maultzsch^1 David Wunderlich^2 Andreas Hirsch^3 Christian Thomsen^1

¹Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

²Zentralinstitut für Neue Materialien und Prozesstechnik, Universität Erlangen-Nürnberg, Dr.-Mack-Str. 81, 90762 Fürth, Germany

³Institut für Organische Chemie, Universität Erlangen-Nürnberg, Henketr. 42, 91054 Erlangen, Germany

We present resonant Raman measurements on carbon nanotubes functionalized with diverse alkyl groups and various degrees of functionalization. From the resonance profiles of the radial breathing mode (RBM) we assign the chiral indices of the tubes [1] in order to study the reactivity as a function of diameter and tube species as has been observed or predicted for several reactants [2,3].

J. Maultzsch et al., Phys. Rev. B 72, 205438 (2005).
 M. Strano et al., Science 301, 1519 (2003).
 S. Niogy et al., Acc. of Chem. Res. 35, 1105 (2002)

16

An analysis of carbon nanotubes wettability before and after oxidation

<u>Simone Musso</u>¹ Stefano Bianco¹ Mauro Giorcelli¹ Alberto Tagliaferro¹ Nicola Pugno² Matteo Pavese³

Wettability of CNTs surface is an important property, governed both by chemical composition and the geometrical microstructure of the contact surface, which

¹Dipartimento di Fisica, Politecnico di Torino, Torino (Italy)

²Dipartimento di Ingegneria Strutturale e Geotecnica, Politecnico di Torino, Torino, Italy

³Dipartimento di Scienza dei Materiali e Ingegneria Chimica, Politecnico di Torino, TORINO (Italy)

can play a key role in CNTs performance during their applications as reinforcements in polymer composites (1), as sensors (2) or as high selective molecular membranes (3). Whereas on the microscopic level (4,5) the wetting behaviour of single CNTs has been studied extensively, the challenge is to understand the wetting behavior at a macroscopic level, when nanotubes are grouped into aligned configurations and the chemical physical manipulation of the properties can greatly facilitate some applications and can also result in some new properties. In this work contact angle measurements have been carried out on different carbon-based materials: graphite and carbon nanotube structures. Thin layers of entangled carbon nanotubes (CNTs) have been considered, together with thick mats of vertically aligned carbon nanotubes (VACNs). In particular, the thick carpets have been investigated both before and after chemical oxidation with nitric sulfuric acid mixture. Tests have been performed using three liquids with different polarity (water, dimethylsulfoxide and diiodomethane). Very high hydrophobicity was observed for the top surface of aligned carbon nanotubes mats, but after oxidation a dramatic reduction of contact angle has been observed, bringing to a hydrophilic behavior. A theoretical calculation of the bulk pore distribution of the material have been modeled to estimate the liquid percolation through oxidized carpets surface.

- 1. Carbon Nanotubes Science and Applications, CRC PRESS, pag. 253 Applications: Composites. Edited by M. Meyyappan
- 2. P. Kim and C. M. Lieber, Science 286 (1999) 2148.
- 3. B.J. Hinds, N. Chopra, T. Rantell, R. Andrews, V. Gavalas, L.G. Bachas, Science 303 (2004) 62.
- $4.\ E.\ Dujardin,\ T.W.\ Ebbesen,\ A.\ Krishnan and M.M.\ J.\ Treacy,\ Adv.\ Mater.\ 10$ (1998), 1472.
- 5. T. Kanyo, Z. Konya, A. Kukovecz, F. Berger, I. Dekany and I. Kiricsi, Langmuir 20 (2004), 1656.

17

Inkjet printing of carbon nanotube transistors on rigid and flexible substrates

<u>Tero Mustonen</u>¹ Jani Maklin¹ Geza Toth¹ Krisztian Kordás¹ Robert Vajtai² Pulickel M. Ajayan³

¹Microelectronics and Materials Physics Laboratories, Department of Electrical and Information Engineering, University of Oulu, P.O. Box 8500, FIN-90014 University of Oulu, Finland

²Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, Troy, New York 12180, USA

 $^3{\rm Department}$ of Mechanical Engineering and Materials Science, Rice University, Houston, Texas 77251-1892, USA

Inkjet printing of carboxyl functionalized single-walled carbon nanotube (SWCNT) on various substrates is investigated. Low and high density networks of SWCNTs,

which have either nonlinear or linear current-voltage characteristics are obtained. The nonlinear, low-density networks are gate-controllable and could be operated as field-effect transistors. The applicability and limitations of inkjet printing technique for micropatterned nanotube thin film generation are discussed.

18

Inkjet printed resistive and chemical-FET carbon nanotube gas sensors

<u>Jani Mäklin</u>¹ Tero Mustonen¹ Niina Halonen¹ Géza Tóth¹ Krisztián Kordás¹ Jouko Vähäkangas¹ Hannu Moilanen² Akos Kukovecz³ Zoltán Kónya³ Zoltán Gingl⁴ Péter Heszler⁵ Henrik Haspál⁵ Robert Vajtaj⁶ Pulickel M. Ajayan⁷

¹Microelectronics and material physics laboratories, University of Oulu, Oulu

Aqueous solutions of carboxyl functionalized single-walled carbon nanotube (SW-CNT) films are deposited on silicon chips by using inkjet printing technique. By varying the film thickness it is possible to obtain low- or high density networks of SWCNTs, having either nonlinear or linear current-voltage characteristics, respectively. The electrical transport in the low-density films is gate-controllable and utilized as chemical field-effect transistor sensors; whereas the high-density SW-CNT networks of Ohmic behavior are used as conventional resistive gas sensors. Chemical sensitivity and selectivity of both types of sensors are studied for nitric oxide (NO), carbon monoxide (CO) and hydrogen sulfide (H_2S) gases.

19

Kekule pattern on conductance images between two STM probes

<u>Takeshi Nakanishi</u>¹ Tsuneya Ando²

The scanning-tunneling-microscopy (STM) is a powerful technique for directly viewing electronic wave functions at the atomic level. Quite recently multi-probe STM was developed. In this paper the conductance image between two STM probes is calculated in an armchair carbon nanotube within a tight-binding model and a

²Laserprobe LP Ltd. Teknologiantie 1, FIN-90570 Oulu, Finland

 $^{^3{\}rm Department}$ of Applied and Environmental Chemistry, University of Szeged, Rerrich B. tér 1, H-6720 Szeged, Hungary

⁴Department of Experimental Physics, University of Szeged, Dóm tér 9, H-6720 Szeged, Hungary

⁵Department of Optics and Quantum Electronics, University of Szeged, Dóm tér 9, H-6720 Szeged, Hungary

 $^{^6 {\}rm Rensselaer}$ Nanotechnology Center, Rensselaer Polytechnic Institute, Troy, New York 12180, USA

⁷Department of Mechanical Engineering and Materials Science, Rice University, Houston, Texas 77251-1892, USA

¹AIST, Tsukuba

²Tokyo Inst. Tech., Tokyo

realistic model for STM probes [1]. We show that a Kekule-type pattern usually appears due to interference of states at K and K points except in special cases. In the calculation, a left STM probe is fixed at several points and a right probe is continuously swept over the wide region. The Kekule-type pattern peak usually appears in the calculated conductance. It disappears in special cases where an electron is injected into a single propagating state classified by the parity in the effective-mass scheme.

1 T. Nakanishi and T. Ando, J. Phys. Soc. Jpn. 77 (2008) No. 2.

20

Photoemission Study of Electronic Structures of Fullerene and Metallofullerene Peapods

<u>Yuji Nakayama</u>¹ Shinichiro Fujiki¹ Yasuharu Hirado¹ Hidetsugu Shiozawa² Hiro-yoshi Ishii¹ Tsuneaki Miyahara¹ Yutaka Maniwa¹ Takeru Kodama¹ Yoji Achiba¹ Hiromichi Kataura³ Masashi Nakatake⁴ Tomohiko Saitoh⁵

¹Tokyou Metroporitan University, 1-1 Minami-Ohsawa, Hachioji, Tokyo 192-0397, Japan

²IFW Dresden, Helmholtzstrabe, 20Germany, Germany

³AIST, 1-1-1 Higashi, Tsukuba 305-8562, Japan

⁴HiSOR, 2-313 Kagamiyama, Higashi-Hiroshima, Hiroshima 739-0046, Japan

⁵Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8651, Japan

We have investigated the electronic structures of C_{70} fullerenes and metallofullerenes (MFs) encapsulated in single-wall carbon nanotubes (SWCNTs), the so-called fullerene peapods (C_{70} @SWCNTs) and metallofullerenes peapods (R@ C_{82} @SWCNTs R= Gd, Dy, La), using photoemission spectroscopy. The photoemission spectra of encapsulating C_{70} and MFs are obtained by subtracting the spectrum of the pristine SWCNTs from those of the corresponding peapods. The electronic structure of encapsulating C_{70} is similar to that of C_{70} film. On the other hand, the energy position of the singly occupied molecular orbital (SOMO) in encapsulating La@ C_{82} is shifted by 0.14eV toward the Fermi energy (E_F), compared with that in La@ C_{82} film. In addition, from detailed analyses of the Gd and Dy 4d-4f resonant photoemission spectra, we estimated the effective Gd and Dy valences of MFs@SWCNTs to be 3.0 and 2.9, respectively.

Entanglement in P@C₆₀ encapsulated in a solid state matrix

Boris Naydenov¹ J. Mende² W. Harneit³ M. Mehring¹

- 12. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany
- ²Deutsches Zentrum für Luft- und Raumfahrt (DLR), Pfaffenwaldring 38-40, Stuttgart, Germany
- ³Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, Berlin, Germany

This contribution concerns quantum information aspects in fullerenes. In particular we present here the preparation of pseudo-pure states and pseudo-entanglement in the coupled electron-nucleus system $P@C_{60}$ (S=3/2 and I=1/2) encapsulated in a solid state matrix. In this system the degeneracy of the high electron spin is lifted, allowing transition selective excitation. Density matrix tomography and phase rotations are applied for detecting pure states and entanglement.

22

Sidewall functionalization of HiPCo nanotubes in toluene

 $\underline{\rm Katalin~Nemeth}^1$ Ferenc Borondics 1 Emma Jakab 2 Aron Pekker 1 Katalin Kamaras 1 Sandor Pekker 1

- ¹Research Institute for Solid State Physics and Optics, Budapest
- ²Institute of Materials and Environmental Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Budapest

In this study we present the synthesis of hydrogenated and alkyl functionalized single-walled carbon nanotubes (SWNTs). The presented reductive functionalization scheme consist of two major steps, the formation and the reaction of the formed carbanions, respectively. In our case carbanions were formed via K intercalation, methanol was used for hydrogenation, and butyl iodide for butylation in anhydrous toluene. Potassium also has an important role in the exfoliation of the nanotube bundles, thus providing a higher yield. The main reaction product is the hydrogenated or alkylated SWNT, but different side reactions are also present, such as hydrogen evolution in case of methanol, and dialkane fomation in case of alkyl halide reagents. The composition of the produts was determined by thermogravimetry-mass spectrometry. The functionalized nanotubes were characterized by Raman and wide-range optical spectroscopy, in order to establish the changes in electronic structure and to investigate diameter and chiral selectivity of the reactions.

Current Filamentation in C60 Diodes through Double Injection

Philipp Stadler¹ Anita Fuchsbauer¹ Almantas Pivrikas¹ <u>Helmut Neugebauer</u>¹ N. Serdar Sariciftci¹ Gebhard J. Matt² Guillaume Goncalves² Dieter Meissner² Thomas Fromherz³ Mujeeb Ullah³ Helmut Sitter³ Günter Hesser⁴

¹LIOS, Physical Chemistry, Johannes Kepler University Linz, Austria

Charge transport in fullerene films is heavily influenced not only by impurities but also by the film morphology [1]. The current-voltage characteristics (IVs) of evaporated C60 thin film diodes follow the space charge limited current (SCLC) theory. Under certain conditions - when using a non-metallic hole injector (PEDOT:PSS) and homogeneous, pure C60 films - deviations from the SCLC behaviour are obtained. The fullerene diodes exhibit voltage instabilities (S-shape IV characteristics) at low temperatures (below 200 K) and at high current densities [2,3]. The instabilities are reversible and correspond to effects, called "Ovonic switches", described with certain non-crystalline inorganic semiconductors [4]. Following this description, charge transport in C60 is influenced by trapping of electrons and holes. We suggest that due to double injection and charge trapping near the electrodes conductive filaments in the fullerene bulk phase are formed, influencing the current flow and causing the voltage instability. We present systematic IV-characteristics of Ovonic switches in C60 diodes at various temperatures. Additionally, morphology studies of C60 films grown by thermal evaporation onto PEDOT:PSS are shown. Cross sectional transmission and scanning electron microscopy studies are presented as well as monitoring of the growth process probed with atomic force microscopy.

- K. Rikitake, T. Akiyama, W. Takashima, K. Kaneto, Synth. Met., 86, 2357 -2358 (1997)
- 2 G. J. Matt, T, Fromherz, N. S. Sariciftci, Appl. Phys. Lett. 84, 1570-1573 (2004)
- 3 G. J. Matt, T. Fromherz, H. Neugebauer, N. S. Sariciftci, CP786, Electronic Properties of Novel Nanostructures, 530 533 (2005)
- 4 N. F. Mott, Contemp. Phys., 10 125-138 (1969)

²Upper Austrian University of Applied Sciences, Campus Wels, Austria

³Institute for Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria

⁴Technische Service Einheit (TSE), Johannes Kepler University Linz, Austria

Observation of a Quantum Phase Transition in a single-molecule Quantum Dot

 $\underline{ROCH\ Nicolas}^1$ FLORENS Serge 1 BOUCHIAT Vincent 1 WERNSDORFER Wolfgang 1 BALESTRO Franck 1

¹Neel Institute, Nanosciences department, Grenoble

Quantum criticality is the intriguing possibility offered by the laws of quantum mechanics when the wave function of a many-particle physical system is forced to evolve continuously between two distinct, competing ground states. This phenomenon, often related to a zero-temperature magnetic phase transition, can be observed in several strongly correlated materials such as heavy fermion compounds or possibly high-temperature superconductors, and is believed to govern many of their fascinating, yet still unexplained properties. In contrast to these bulk materials with very complex electronic structure, artificial nanoscale devices could offer a new and simpler vista to the comprehension of quantum phase transitions. This long-sought possibility is demonstrated by our work in a fullerene molecular junction, where gate voltage induces a crossing of singlet and triplet spin states at zero magnetic field. Electronic tunneling from metallic contacts into the! C_{60} quantum dot provides here the necessary many-body correlations to observe true quantum critical behavior. With our work, we demonstrate that C_{60} QDs in nanoscopic constrictions present the two key ingredients for observing quantum phase transitions: a gate-tuning of the singlet-triplet gap at zero magnetic field, and a single screening channel. This experiment constitutes thus a further step for the realization in Qds of fundamental many-body effects relevant for bulk correlated materials, and opens also new possibilities for the precise control of spin states in nanostructures containing few electrons.

I will present a full experimental study of transport measurements on a C_{60} QD, as a function of bias voltage (V_b) , gate voltage (V_g) , temperature (35mK to 20K), and magnetic field (0 up to 8 Tesla). A scaling analysis of our conductance measurements reveals the nature of the quantum critical point!, in the vicinity of which a surprisingly rich interplay of severa ondo effects occurs. These include the underscreening of a spin S=1 state on the triplet ground state side, a fully developed inverse Kondo dip on the singlet ground state side, as well as complex non-equilibrium Kondo features on both sides of the transition.

Electron beam induced electronic transport in vanadium oxide nanotubes

C. ODwyer¹ C. Clavijo² V. Lavayen³ C. M. Sotomayor Torres⁴

¹Tyndall National Institute, University College Cork, Cork, Ireland

²Dept. of Mathematics and Computer Science, Faculty of Electrical Engineering, University of Twente, The Netherlands

³UFMG, Departamento de Fisica, Av. Antonio Carlos, 6627, Belo Horizonte, 30123-970, MG, Brazil

⁴Institute for Research and Advanced Studies, ICREA, 08010 Barcelona, Spain and Catalan Institute of Nanotechnology, Edifici CM7, Campus Universitat Autonoma de Barcelona, 08193 Bellaterra (Barcelona), Spain

The fabrication of synthetic nanotubes does not require high-resolution lithography, which makes them attractive as components of nanoscale electrical devices. In addition, field-effect transistors (FETs) from individual nanotubes have been reported. Inorganic materials like WS₂ nanotubes, silicon nanowires, or vanadium pentoxide nanotubes as well as molecules such as DNA, have garnered increasing importance in this regard. In the present study, we employ vanadium pentoxide (V_2O_5) nanotubes as effective conducting tubular wires with thicknesses of molecular dimensions. The electrical transport through alkyl monoamine-intercalated V₂O₅ nanotubes can be effectively modulated by the potential of a gate electrode, representing a new type of nanoFET based on hybrid organic-inorganic nanotubes. A combination of nanoimprint lithography (NIL) and photo-lithographic techniques were used to produce nanometer-sized interdigitated electrodes with channel lengths of 100 nm [1-3]. V₂O₅ nanotubes, formed by mild hydrothermal treatment of monoamine intercalated laminar V_2O_5 xerogel [4], were drop-cast on the electrode surface utilizing the negatively charged nanotube affinity to control the adsorption process.

Electron beam induced current (EBIC) measurements and voltage contrast (VC) measurements were found to be suitable and applicable techniques for alkyl monoamine-intercalated V_2O_5 nanotubes and will be shown to map the electronic transport properties with a 10 nm spatial resolution. The findings comprise the fabrication of solution processable V_2O_5 nanotube-channelled FETs by patterning of interdigitated structures by NIL and selective adsorption of the nanotube channels. Electrical characterization of the FET structures evidences a reduced polaron hopping activation energy to those from nanofiber [5] and nanowire-based structures [6], linked to the absence of transport barriers at inter-tube contacts and the nanotube-channelled structure exhibits an n-type enhancement mode. Finally, evidence is presented for a thermally driven small polaron-hopping conduction mechanism as a function of vanadium valency.

 A.P. Kam, J. Seekamp, V. Solovyev, C. Clavijo Cedeno, A. Goldschmidt, C.M. Sotomayor Torres, *Microelec. Eng.* 2004 73-74, 809.

- 2 C.M. Sotomayor Torres, S. Zankovych, J. Seekamp, A.P. Kam, C. Clavijo Cedeno, T. Hoffmann, J. Ahopelto, F. Reuther, K. Pfeiffer, G. Bleidiessel, G. Gruetzner, M.V. Maximov, B. Heidari, Mat. Sci. Eng. C 2003 23, 23.
- 3 C. Clavijo Cedeno, J. Seekamp, A.P. Kam, T. Hoffmann, S. Zankovych, C.M. Sotomayor Torres, C. Menozzi, M. Cavallini, M. Murgia, G. Ruani, F. Biscarini, M. Behl, R. Zentel, J. Ahopelto, Microelec. Eng. 2002 61–62, 25.
- 4 V. Lavayen, C. ODwyer, S.B. Newcomb, M.A. Santa Ana, E. Benavente, G. Gonzalez, C.M. Sotomayor Torres, phys. stat. sol. (b) 2006 243, 3285.
- 5 G.T. Kim, J. Muster, V. Krstic, J.G. Park, Y.W. Park, S. Roth, M. Burghard, Appl. Phys. Lett. 2000 76, 1875.
- 6 J. Park, E. Lee, K.W. Lee, C.E. Lee, Appl. Phys. Lett. 2006 89, 183114.

Magnetotransport on single-walled carbon nanotubes and graphene

Dirk Obergfell¹ Miroslav Haluška² Siegmar Roth¹

Single-walled carbon nanotubes (SWNTs) were produced by the arc-discharge method using non-magnetic catalysts [1], subsequently adsorbed from dispersion onto Si/SiO₂ substrates and contacted in field-effect transistor configuration. Graphene flakes on top of Si/SiO₂ chips were fabricated utilizing the established micromechanical cleavage method [2,3] and contacted by standard e-beam lithography. Both SWNTs and graphene layers were investigated by 2-probe magnetotransport measurements with external magnetic fields applied in different directions. As anticipated, no clear effects were observed for the graphene flakes at in-plane magnetic fields, whereas signatures of Hall and Quantum Hall effect became visible for perpendicular magnetic fields. Some SWNTs exhibited up to 10% negative magnetoresistance for axially oriented magnetic fields, in contrast no effects were observable for external magnetic fields perpendicular to the nanotube axes. The SWNT magnetotransport results will be discussed in terms of Aharanov Bohm phase shift and weak localization.

References:

- 1. Haluška, M. et al. Synthesis of SWCNTs for C₈₂ peapods by arc-discharge process using nonmagnetic catalysts. phys. stat. sol. (b) 243, 3042-3045 (2006).
- 2. Novoselov, K. S. et al. Two-dimensional atomic crystals. Proc. Natl. Acad. Sci. USA **102**, 10451-10453 (2005).
- 3. Novoselov, K. S. et al. Electric Field Effect in Atomically Thin Carbon Films. Science 306, 666-669 (2004).

¹Max Planck Institute for Solid State Research, Stuttgart, Germany

²Micro and Nano Scale Engineering, Technical University of Eindhoven, the Netherlands

CARBON NANOTUBE-BASED OPTICAL MEDIA WORKING IN SPECTRAL RANGE 1.0 - 2.5 MICROMETERS

<u>Elena D. Obraztsova</u>¹ Alexander I. Chernov¹ Anatoly S. Lobach² Marina Y. Zavodchikova³ Albert G. Nasibulin³ Esko I. Kaippinen³

¹A.M. Prokhorov General Physics Institute, RAS, 38 Vavilov street, 119991, Moscow, Russia

²Institute of Problems of Chemical Physics, RAS, 142432, Chernogolovka, Russia ³NanoMaterials Group, Lab. of Physics and Center of New Materials, Helsinki, University of Technology, PO Box 1000, 02044, Espoo, Finland

Due to a growing interest to the optical media incorporating single-wall carbonnanotubes (SWNTs) being able to work in IR spectral range as ultrafast modulators of laser beams [1], in this work we have performed a systematic comparative study of 3 types of SWNTs: HiPCO, arc and ferrocene-CO-CVD [2]. The Raman and UV-VIS-NIR absorption spectra have been measured in detail. The media have been taken in form of thin polymer films (4-20 mkm) incorporating SWNTs, or thin SWNT films deposited onto quartz substrates. The optical losses of different types of the media were controlled and kept comparable. The measurements have shown that the absorption bands of these 3 materials, with a slight overlapping, have covered completely a spectral range from 1 mkm to 2.5 mkm. Namely, the band center for HiPCO SWNTs was at 1200 nm, for arc nanotubes it was at 1750 nm and for the ferrocene-CO-CVD nanotubes it was at 2130 nm. The band maximum positions have been used to estimate the average nanotube diameters. They were 1.0 nm, 1.4 nm and 1.8 nm for HiPCO, arc and the ferrocene-CO-CVD nanotubes, correspondingly. These values have coincided very well with the estimations based on the positions of the Raman breathing modes for the same materials. Up to now the efficiency of SWNTs as saturable absorbers have been demonstrated up to 1.93 mkm (thullium fiber laser) [3]. A possibility to use the nanotubes working in the range 2.0-2.5 mkm is very promising for realization of the ultra-short pulse generation in much wider class of solid state lasers, for instance, in the holmium fiber laser working at wavelength 2.1 mkm.

it The work is supported by RFBR 07-02-91033-AF, FP7-033350 and by the Academy of Finland.

- 1 A.V. Tausenev, E.D. Obraztsova, A.S. Lobach et al., Quantum Electronics 37 (2007) 847.
- 2 A. Moisala, A.G. Nasibulin, D.P. Brown, H. Jiang, L. Khriachtchev and E. I. Kauppinen, Chemical Engineering Science 61 (2006) 4393.
- 3 M.A. Solodyankin, E.D. Obraztsova, A.V. Lobach et al., Optics Letters 2008 (submitted).

STATISTICAL ANALYSIS OF ATOMIC FORCE MICROSCOPY AND RAMAN SPECTROSCOPY DATA FOR ESTIMATION OF GRAPHENE LAYERS NUMBER

 $\underline{\text{Ekaterina A. Obraztsova}^1}$ Alexander V. Osadchy² Elena D. Obraztsova² Serge Lefrant³ Igor V. Yaminsky¹

¹Physics department, M.V.Lomonosov Moscow State University, Moscow

²A.M. Prokhorov General Physics Institute, RAS, 38 Vavilov street, 119991, Moscow, Russia

³Institut des Materiaux Jean Rouxel, UMR 6502, 2 rue de la Houssiniere, B.P. 32229, 44322, Nantes, Cedex3 - France

In this work we present the results on preparation and analysis of structural and electronic properties of n-layer graphene structures. The samples were prepared by a micro-cleavage technique [1]. The obtained samples contained several n-layer graphene flakes onto silicon oxide surface. To estimate the number of layers in each flake the numerous atomic force microscopy (AFM) measurements have been performed in different points of flakes. The array of the thickness values estimated by AFM have exhibited a set of maxima: 0.7 nm, 1.1 nm, 1.4 nm, 1.7 nm, 2.1 nm etc. These values correspond ideally to the one-, two, three-, etc. layered graphene. To check an accuracy of AFM estimations the same flakes have been studied by two-phonon Raman spectroscopy known as a tool, being sensitive to the number of graphene layers [2]. The spectra have been registered with the different excitation wavelengths. The electronic structure of n-layered graphene has been modeled using the density functional technique. An estimation of the number of graphene layers in the different flakes was based on the parameters of components observed in two-phonon Raman spectra matched to the possible electronic transitions calculated. Perfect correspondence between the estimations made by AFM and Raman techniques have been obtained.

This work was supported by RFBR-07-02-01505 and INTAS 05-109-4966.

- 1 K.S. Novoselov et al., Science 306 (2004) 666.
- 2 A.C. Ferrari, J.C. Meyer et al., Phys. Rev. Lett. 97(2006)187401.

29

Optical Band Gap Modification of Single-Walled Carbon Nanotubes by Encapsulated Fullerenes

Toshiya Okazaki¹ Shingo Okubo¹ Takeshi Nakanishi¹ Soon-Kil Joung¹ Takeshi Saito¹ Minoru Otani² Susumu Okada³ Shunji Bandow⁴ Sumio Iijima¹

¹Research Center for Advanced Carbon Materials, AIST, Tsukuba

²Institute for Solid State Physics, University of Tokyo, Tokyo

³Institute of Physics and Center for Computational Sciences, University of Tsukuba, Tsukuba

⁴Department of Materials Science and Engineering, Meijo University

We report optical band gap modifications of single-walled carbon nanotubes (SW-NTs) upon C60 insertions by using photoluminescence (PL) and the corresponding excitation spectroscopy. The shifts in optical transition energies strongly depend on the tube diameter and the "2n+mfamily type, which can be explained by the local strain and the hybridization between the nanotube states and the C60 molecular orbitals. The present results provide possible design rules for nanotube-based heterostructures having a specific type of electronic functionality.

30 ELECTRONIC STRUCTURE AND ELECTROCHEMICAL CHARACTERISTICS OF ONION-LIKE CARBON MATERIALS

<u>Alexander V Okotrub</u>¹ Lyubov G Bulusheva¹ Evdokia G Bushueva¹ Vladimir V Kuznetsov²

¹Nikolaev Institute of Inorganic Chemistry SB RAS, Siberian Branch Russian Academy of Science, Novosibirsk

²Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Nanodiamonds (ND) prepared by a detonation method, have been annealed in a high vacuum at temperatures 1420, 1600, 1900 and 2140 K. Transmission electron microscopy showed the rearrangement of ND surface into 2-3 graphitic layers when temperature increases up to 1420 K, the nanoparticles produced at 1800 K have quasi-spherical onion-like form with layer spacing close to the graphite one. The final stage of ND annealing yields multilayered graphitic polyhedral particles having a hollow inner space. X-ray emission and X-ray absorption spectroscopy detected the difference in the electronic state of carbon shells generated below 2140 K and that of graphite. An intense maximum found in the high-energy region of the CKa spectrum indicated significant localization of weakly bonding electrons in onion-like carbon. Quantum-chemical calculations on the carbon models revealed this localization might result from defects in the curved graphitic networks, namely, the holes which appear through a deficit of surface atoms of ND that are required to form an ideal spherical shell. The supercapacitor characteristics of the samples have been investigated in different electrolytes. It was found that in the considered set of the samples the onion-like carbon particles possess by higher capacitance both in acidic 30 F/g and in alkaline 15 F/g electrolytes.

$\it pi$ Electron Spectrum of Finite-Size Honeycomb Lattices: Exact Versus Approximate Results

Lyuba Malysheva¹ Sven Stafström² Alexander Onipko³

¹Division of Quantum Electronics, Bogolyubov Institute for Theoretical Physics, 03680, Kyiv, Ukraine

 2 Department of Physics, IFM, Linköping University, S-581 83 Linköping, Sweden 3 Division of Theory and Similation of Plasma Processes, Bogolyubov Institute for Theoretical Physics, 03680, Kyiv, Ukraine

It is shown that in the tight-binding approximation, the π electron spectrum of honeycomb lattices framed by two armchair- and two zigzag-shaped boundaries is determined by the 2D-graphite dispersion relation supplemented by the generalized Lennard-Jones equation. These two relations give the exact solution of the spectral problem for a graphene sheet containing an arbitrary number of N (oligo) polyacenes coupled to each other by N C-C bonds. Applications of the developed approach are exemplified by a detailed analysis of armchair and zigzag graphene ribbons. It is argued that the description of edge states of zigzag ribbons on the basis of Dirac equation is correct qualitatively but not quantitatively. The spectrum and wave functions of these states are represented in the form of analytic relations supported by exact numerical calculations.

32

Diameter selectivity of nanotube sidewall functionalization probed by optical spectroscopy

Aron Pekker¹ Katalin Kamaras¹ David Wunderlich² Andreas Hirsch²

¹Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary

 2 Institute for Organic Chemistry, University of Erlangen-Nürnberg, Henkestr. 42, 91054 Erlangen, Germany

We present here wide range optical measurements on functionalized HiPCO nanotubes [1]. In the infrared spectum of HiPCO nanotubes the peaks show fine structure, where the separate peaks are related to nanotubes with different diameters. This gives us the opportunity to investigate the possible diameter dependence of the functionalization efficiency.

We measured several samples functionalized with butyl sidegroups with different concentration [2]. In order to access the widest possible range on the same sample, we prepared self-supporting thin films from these materials. From the transmission spectrum optical conductivity was calculated by Kramers-Kronig transformation and fitted by Drude - Lorentz oscillators.

Comparing the results we show that the nanotubes with smaller diameters are affected more easily by functionalization.

- P. Nikolaev, M. J. Bronikowski, R. K. Bradley, F. Rohmund, D. T. Colbert, K. A. Smith, R. E. Smalley, Chemical Physics Letters, 313, (1,2), 1999
- 2 R. Graupner, J. Abraham, D. Wunderlich, A. Vencelova, P. Lauffer, J. Röhrl, M. Hundhausen, L. Ley, A. Hirsch, J. Am. Chem. Soc., 128, 2006

Ressonance Raman Excitation Energy Map and High Resolution Transmission Electron Microscopy of hundreds of (n,m) Single Wall Carbon Nanotubes

Pedro B C Pesce¹ Paulo T Araujo¹ Stephen K Doorn² Pasha Nikolaev³ Ado Jorio¹ Departamento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brasil

²Chemistry Division, Los Alamos National Laboratory, Los Alamos, USA ³ERC/NASA-JSC, Houston, Texas, USA

In this work we measure the Raman spectra of a SWNT sample with a wide diameter distribution - 1nm to 6nm - with closely spaced laser lines over the 1.26eV to 2.71eV energy range and did a thorough analysis of the observed features. The most intense peaks are assigned to the scattering of light by a single RBM phonon in ressonance with the well-known excitonic E_{ii} transitions. Comparison of the Raman map with the diameter distribution of the sample, obtained from HRTEM measurements of 395 different nanotubes allows us to determine the diameter dependence of the RBM cross section. Furthermore, a number of weaker features are identified with different mechanisms, such as the RBM overtone and cross polarized transitions.

34

A detailed comparison between precursor based and CVD-grown DWCNTs

<u>Rudolf Pfeiffer</u>¹ Herwig Peterlik¹ Hans Kuzmany¹ Ferenc Simon² Karin Pressl³ Peter Knoll³ Morinobu Endo⁴

Recently, we studied the detailed transformation dynamics of C_{60} and ferrocene (FeCp₂) filled SWCNTs into DWCNTs. It turned out that these starting materials give rise to two different growth processes, namely a non-catalytic fusion of the fullerenes in the first case and a catalytic growth of the inner tubes in the latter case. Even for the same starting SWCNTs material these two processes resulted in different inner-outer tube pair distributions.

In this contribution we present a thorough comparison of DWCNTs directly grown from a CVD process and DWCNTs produced from the above two starting materials.

¹Fakultät für Physik, Universität Wien, Wien, Austria

²Budapest University of Technology and Economics, Budapest, Hungary

³Karl-Franzens Universität Graz, Graz, Austria

⁴Shinshu University, Nagano, Japan

We studied the samples with Raman spectroscopy for excitations from IR to UV and with x-ray diffraction. It turned out that the CVD grown tubes are more similar to the FeCp₂ based DWCNTs with respect to the inner-outer tube pair distribution. However, regarding the Raman frequencies and the Raman lines widths all three samples are comparable. Finally, an anomalous dispersion for the D-line and for its overtone was observed for the inner tubes in a similar way for the peapod grown and for the CVD grown tubes.

Work supported by FWF project I83-N20 (ESF IMPRESS).

35

Surface enhanced Raman spectroscopy of liquid crystal 8CB using chip structures

 $\underline{\mathrm{W.~Plank}^1}$ M. Hulman² H. Kuzmany¹ A. Köck² K. Roppert² A. Kukovecz³ J. Krenn⁴ R. Bischof⁴

Molecular nanostructures are excellent systems to study surface enhanced Raman scattering (SERS), since monolayers or sub-monolayers are expected to provide maximum scattering enhancement. The SERS enhancement is due to a plasma induced field enhancement by metallic nanoparticles. By this effect the Raman response of molecules in the immediate neighborhood of the particles can be dramatically increased.

We investigated the SERS effect of Ag colloides on glas substrates and on lithographically produced nanostructures of gold and aluminium on silicon and ITO glass.

For testing extremely thin layers (monolayers and submonolayers) of 4,4 Octylcyanobiphenyl (liquid crystal 8CB) were prepared. The observed enhancement for 8CB on Ag colloides was about 10^3 .

Enhancement factors for the lithographic structures were initially below 100. To increase the enhancement the Au nanostructures were coated with a 20 nm thick Ag-layer. Optimisation of the Ag nanoparticle geometry was investigated as an alternative SERS improvement routine. The viability of the chip structures for multiple usage was tested. The experimental analysis was supported by calculations of the SERS cross-section for different structure geometries.

This work was supported by the Austrian Nanoinitiative, Projekt 810401/S14

¹Faculty of Physics, University of Vienna, Austria

²Austrian Research Center

³Faculty of Science, University of Szeged

⁴Institute of Physics, Karl Franzens University Graz, Austria

Monitoring several environmental parameters at once: multi-level modelling of carbon-nanotube-based sensors

 $\underline{\mathrm{Yann}\ \mathrm{Pouillon}^1}$ Juan María García Lastra
¹ Angel Rubio¹

¹European Theoretical Spectroscopy Facility, Universidad del PaÃs Vasco UPV/EHU, Donostia-San SebastiÃ;n

The SANES (Self-Adjusting Nano-Electronic Sensors) project aims at designing, building, and characterizing integrated multifunctional nanotube-based sensor micromodules, in order to monitor simultaneously several environmental parameters, like temperature, pressure, and gas concentration, in various conditions. Potential applications range from security to medicine, covering communication and environmental issues as well.

Experimental challenges involve manipulating and contacting very small systems reliably, measuring and processing low-amplitude and extremely noisy signals, as well as choosing adequate molecules to functionalize the CNTs, in order to enhance both sensitivity and selectivity. A better theoretical understanding is clearly needed for all this, in which the requested accuracy defines the parts of the systems that can be addressed.

In order to provide the experimentalists with a valuable insight into the properties of these CNTs, to speed-up the process of selecting functional molecules, and to meet the challenges brought by the sizes of the systems involved, we are thus conducting series of calculations of their structural, electronic, and transport (I/V characteristics) properties at multiple levels: empirical, tight-binding, and *ab initio*. Some emphasis is put on the role of water.

37

Magnetic-field effects on heavily disordered graphene

Stephen R. Power¹ Mauro S. Ferreira¹

¹School of Physics, Trinity College Dublin, Dublin 2, Ireland.

The electronic structure of graphene has been much studied recently, with the obvious intention of exploring the linearity of its dispersion around the Fermi level. External magnetic fields are known to affect the electronic structure of a material by the introduction of Landau levels and have been in focus recently. Disorder is also known to affect the electronic energy level distribution but is often ignored in many calculations. Here we consider the effect of magnetic fields on the electronic structure of graphene in the presence of strong disorder. Based on the nearest-neighbour tight-binding model, we consider randomly distributed substitutional and adsorbed impurities. The magnetic field is accounted for by the Peierls phase method. Configurational averaging is performed both by brute-force methods and

using the Coherent Potential Approximation. A systematic study is carried out by varying the magnetic field strength, the impurity concentration and the nature of the impurity.

38

Exciton transfer and propagation in carbon nanotubes studied by near-field optical microscopy

<u>Huihong Qian</u>¹ Carsten Georgi¹ Alexander A. Green² Mark C. Hersam² Lukas Novotny³ Achim Hartschuh¹

¹Department Chemie und Biochemie, Ludwig-Maximilians-Universitaet, Muenchen ²Department of Materials Science and Engineering, Department of Chemistry, Northwestern University, Evanston, Illinois

³The Institute of Optics, University of Rochester, Rochester, New York 14627, USA

Single-walled carbon nanotubes feature unique electronic properties making them ideal candidates for ultra-high density devices in electronics, photonics and optoelectronics. Photoluminescence (PL) from semiconducting carbon nanotubes results from exciton recombination. We use tip-enhanced near-field optical microscopy (TENOM [1-3]) as a tool to visualize PL properties on a nanometre length scale. Near-field PL and topography images of a single nanotube bundle reveal the presence of two semiconducting nanotubes with different chiralities having an internanotube spacing ranging from 1 to 4 nm. PL from the large band gap nanotube was observed with unexpectedly high intensities varying spatially due to distance dependent inter-nanotube energy transfer. Efficient transfer is found to be limited to a few nanometres because of competing fast non-radiative relaxation and can be explained in terms of electromagnetic near-field coupling. Towards the end of nanotube, PL decay is observed on a length scale of 15-40 nm that is attributed to exciton propagation followed by additional non-radiative relaxation at the nanotube end.

- 1 Hartschuh, A. et al, Nano Lett. 5, 2310-2313 (2005).
- 2 Hartschuh, A. et al, Phys. Rev. Lett. 90, 095503-095506 (2003).
- 3 Kawata, S. and Shalaev, V. M., editor. Tip enhancement. Advances in Nano-Optics and Nano-Photonics. Elsevier, Amsterdam, (2007).

วด

Electrochemical Functionalization of SWNT bundles in acid and salt media as observed by Raman and X-ray Photoelectron Spectroscopy

Peter M. Rafailov¹ Christian Thomsen² Ursula Dettlaff-Weglikowska³ Siegmar Roth³ Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria ²Institut für Festkörperphysik, Technische Universität Berlin, Germany

³Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We carried out electrochemical functionalization of single-walled carbon nanotube mats (buckypaper) in HCl and KCl aqueous solutions by exposing them to electrochemical potentials above the Cl⁻ oxidation potential and high Faradaic currents. Formation of C-Cl covalent bonds was established by X-ray Photoelectron Spectroscopy (XPS). Combining results from Raman, XPS and conductivity measurements, we find a significantly higher degree of functionalization in the HCl solution as compared to the KCl one. We also discuss the impact of electrochemical doping and functionalization on the morphology and the conductivity of the SWNT bundles.

40

Comparative photoluminescence of three Er-doped trimetallic nitride template fullerenes

R. Rahman¹ G. Dantelle¹ K. Porfyrakis¹ A. Tiwari¹ A. Ardavan² G.A.D. Briggs¹ Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, UK

 $^2\mathrm{QIPIRC},$ Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK

Endohedral fullerenes, where atoms are trapped inside the carbon cage, are showing great promise as candidates for quantum information processing (QIP) with electronic spins, in particular because the shielded atoms inside the cage often exhibit long decoherence times and relatively pure states. One of the great challenges for QIP with such materials is the detection limit for current electron spin resonance (ESR) techniques, which is around 10^{12} spins. One possible way to significantly lower this limit is to use light detection of magnetic states. Erbium-scandium trimetallic nitride template fullerenes, $Er_xSc_{3-x}N@C_{80}$ with x=1, 2 or 3, have Er^{3+} ions emitting around 1.500nm where the C_{80} cage is transparent. The photoluminescence (PL) spectra of the three Er-Sc TNT fullerenes were taken around 1500nm at various temperatures. The PL peaks intensities were used to compare the luminescence of the different TNT fullerenes. We show that there is no linear relationship between the erbium content and the intensity of the emission peaks when we compare the different TNT fullerenes. Among the three compounds, $ErSc_2N@C_{80}$ seems to have the strongest 1500nm luminescence intensity with respect to the erbium content. $ErSc_2N@C_{80}$ is also spin active, which makes it a very interesting potential candidate for optical readout of spin states.

Electronic hybrid structures formed by carbon nanotubes and metallic nanowires

Nitesh Ranjan¹ Michael Mertig²

 $\overline{\ }$ Institute of Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden

Carbon nanotubes and solid-state nanowires are considered to be the most promising candidates for future nanoelectronics. Carbon nanotubes exists as both metallic and semiconducting ones. While metallic carbon nanotubes can be used as interconnects in the integrated circuits, semiconducting nanotubes can be used as nanoelectronic devices such as field-effect transistors[1]. Metallic nanowires can now be directly grown between the electrodes by dielectrophoresis having one-dimensional electrical properties similar to metallic carbon nanotubes [2].

We here present an ingenious method to combine carbon nanotubes with metallic nanowires in nanoelectronic circuits. In this method, the nanotubes are first deposited between micro-fabricated electrodes by dielectrophoresis. Thereafter, the formed nanotube bridges were cut either by burning them electrically or by mechanical rupture by means of AFM tips. Burning was achieved by passing excessively high current through the carbon nanotubes which finally burnt them locally. AFM cutting was obtained by moving the AFM tip over the nanotubes bridges with high loading force. The broken bridges were then joined by metallic palladium nanowires using dielectrophoretic deposition from a palladium salt solution. The obtained nanoelectronical structures were imaged by AFM and SEM. Room temperature I-V characteristics were taken of pure carbon nanotubes, during the burning process and of the hybrid structures formed after coupling CNTs with metallic nanowires. We demonstrate that the developed method can be used to restore the functionality of broken nanoelectronic circuits, and to unravel novel electronic properties of low-dimensional hybrid structures.

- 1 S. Taeger, M. Mertig: Self-assembly of high-performance multi-tube carbon nanotube field-effect transistors by ac dielectrophoresis, International Journal of Materials Research 98, 742-748 (2007).
- 2 N. Ranjan, H. Vinzelberg, M. Mertig: Growing one-dimensional metallic nanowires by dielectrophoresis. Small 2, 1490-1496 (2006).

42

Ex-situ Synthesized Nickel Nanoclusters: easy-to-use Carbon Nanotube pre-

Chandramohan George¹ Maria Teresa Parodi¹ Alberto Ansaldo² Ermanno Di Zitti¹ Siegmar Roth³ <u>Davide Ricci</u>²

 $^1\mathrm{Dipartimento}$ di Ingegneria Biofisica ed Elettronica, Universit
'a di Genova, Genova - Italy

²Dresden University of Technology, D-01062 Dresden, Germany

One of the key steps in Carbon Nanotube (CNT) synthesis via Chemical Vapour Deposition (CVD) is the preparation of appropriate metal precursors that act as catalysts for CNT growth. The most common approaches for activating the sample surface typically rely on the in-situ preparation of metallic clusters obtained either starting from evaporated thin metal films or from coatings of metallic compounds. In this work we present an alternative approach based on the ex-situ preparation of a suspension of metallic nanoclusters, namely Nickel nanoparticles, that can be used as a precursor ink for the activation of the substrate where CNTs have to be grown. The Nickel nanoparticles (NiNPs) are synthesized ex situ by a hot injection method involving the reduction of Nickelacetylacetone [Ni(acac)₂] with sodium tetrahydridoborate, [NaBH₄], in the presence of oleylamine. The precursor ink is then obtained by dispersing the NiNPs in hexane. NiNPs have shown to be stable for many months, their size has been tuned during synthesis or later via size-selection methods, and their concentration can be changed by several orders of magnitude. We present preliminary results on the growth of CNTs using NiNPs as precursors on flat surfaces such as silicon oxide and also on very high aspect ratio surfaces, i.e. sharpened tungsten wires. Advantages and issues compared to in-situ cluster preparation techniques are discussed.

43

MEMORY EFFECTS IN CARBON NANOTUBE BASED DEVICES

 $\underline{\text{Marcus Rinki\"o}}^1$ Andreas Johansson
¹ Marina Zavodchikova² Jussi Toppari¹ Päivi Törmä²

Carbon nanotube field-effect transistors (CNT-FETs) are proposed as possible building blocks for future nano-electronics. But a challenge there is that they often display some degree of hysteresis in their transfer characteristics. For field-effect transistor this is an undesired feature that causes its output to be unpredictable. This has motivated several studies of finding ways to prevent or remove these tendencies. On the other hand, this opens up new possibilities for using these CNT-FETs as memory elements instead by utilizing the hysteresis. Several studies have shown CNT-FETs with well separated ON and OFF states at zero gate voltage and these states are addressable with positive or negative gate voltage pulses, due to hysteresis. Until now the challenge has been to really understand the source of hysteresis and how to control it, which so far has been reported as a more or less random property among the studied CNT-FETs. The gate insulator film has here a crucial influence on the operation of the CNT-FET. For an effective capacitive coupling between the CNT and the gate electrode, a thin and dielectrically strong

²Istituto Italiano di Tecnologia, Genova - Italy

³Max-Planck-Institut für Festkörperforschung, Stuttgart - Germany

¹University of Jyväskylä

²Helsinki University of Technology

film is required. On the other hand, in order to achieve the desired hysteretic behavior for a non-volatile memory, the gate-nanotube coupling has to include some mobile charges or charge traps within the gate insulator or at some interface in the system. Here we present a novel way of controlling this hysteresis and show results that bring us a bit closer for utilizing carbon nanotubes in the future as memory devices.

44

Graphene layers on silicon carbide studied by Raman spectroscopy

<u>Jonas Röhrl</u>¹ Martin Hundhausen¹ Ralf Graupner¹ Konstantin V. Emtsev¹ Thomas Seyller¹ Lothar Ley¹

¹Technische Physik, Erlangen, Deutschland

We present micro Raman spectroscopy studies of few layer graphene (FLG) which were prepared by annealing of SiC at elevated temperatures. These large domains of FLG are crystalline and oriented with respect to the underlying SiC substrate. The average thickness of the FLG-samples was determined by photoelectron spectroscopy and the local thickness ($2\mu m$ resolution), from the Raman-line shape of the 2D-peak.

Samples with different average thicknesses of FLG were studied. The representative phonon lines in the Raman spectra are the G-peak and the 2D-peak. We find a significant shift of these lines to higher frequency compared to HOPG and exfoliated graphene layers. The phonon-frequency shift is particularly large for a graphene monolayer where it amounts to about $30cm^{-1}$. For this phonon hardening of the epitaxial monolayer on the reconstructed SiC surface we consider two effects: the influences of charge on the Kohn-anomaly, and compressive strain induced in the graphene layer by the underlying substrate.

45

Selective vertically aligned CNT growth in vias using electrodeposition

<u>Ainhoa Romo Negreira</u>¹ P.M. Vereecken² D.J. Cott¹ S. De Gendt³ K. Maex¹ M.M. Heyns⁴

¹KU Leuven Department of electrical engineering, B-3001 Heverlee Belgium

In recent years, carbon nanotubes (CNTs) have stimulated extensive research within the field of semiconductor device fabrication. In the specific case of interconnect application for integrated circuit (IC) technology, CNTs could replace copper because they have lower resistivity and delay, lower dynamic power and better thermal behaviour in vias than copper.

²IMEC Kapeldreef 75, B-3001 Heverlee Belgium

³KU Leuven Department of Chemistry, B-3001 Heverlee Belgium

 $^{^4\}mathrm{KU}$ Leuven Department of Metallurgy and Materials engineering, B-3001 Heverlee Belgium

Crucial factor to reach high quality growth and sufficient packing density is a suitable placement of catalyst species on the surface (and in the vias). Until now, physical vapor deposited (PVD) metal films and metal particle impregnated supports have been used for CNT growth. But they lack control over size, density and location. To address these challenges, we are investigating electrodeposition as an alternative technique for catalyst preparation. This technique offers control over size, density and a high degree of selectivity, which is essential for IC integration. As such, monodispersed sub-nm to nm particles at a predefined location of patterned structures can be achieved. It also offers the possibility of preparing bicatalysts through the alloying of different metals.

In this work, nickel nanoparticles were electrodeposited on semiconductor surface and a metal-like layer, (100) n-type silicon wafer and titanium nitride (TiN) respectively. The deposition parameters (potential, time) dependence was studied. These nanoparticles were very successful for vertically aligned CNT growth. The growth was then compared with PVD films with an equivalent thickness.

Furthermore, in order to demonstrate the selectivity of the technique, nickel nanoparticles were deposited at the bottom of 150 to 300 nm diameter via structures patterned in a SiO2 layer resulting in the high density selective growth of CNTs within the vias. The size and density of the particles achieved inside vias corresponded with the result obtained on blankets, which makes the process totally transferable from blanket to patterned structures.

The nanoparticle sizes and densities were characterized by SEM, TXRF and the CNTs morphology by SEM, TEM and RAMAN spectroscopy.

46

Vibrational properties of semitrimer picotubes: *ab initio* calculations and Raman spectroscopy

 $\underline{\rm Nils~Rosenkranz}^1$ María Machón 1 Rainer Herges 2 Christian Thomsen 1

¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

²Institut für Organische Chemie, Christian-Albrechts-Universität Kiel, Otto-Hahn-Platz 4, 24098 Kiel, Germany

Picotubes are highly symmetric ring-shaped hydrocarbons closely related to very short carbon nanotubes. We study the vibrational properties of the semitrimer picotube and find the structural similarity to the corresponding (3,3) nanotube to be reflected also in the Raman spectra. We identify the symmetries of all prominent Raman modes of semitrimer picotubes by means of polarization-dependent measurements on crystalline samples. Furthermore, the semitrimer molecule has been subject to *ab initio* calculations, the results of which agree excellently to the experimental data. By comparing experiment and theory, we can assign phonon eigenvectors to all main Raman peaks.

Dimensionality effects in the optics of BN nanostructures: applications for optoelectronic devices

Claudio Attacalite¹ Angel Rubio¹ Ludger Wirtz² Andrea Marini³

¹European Theoretical Spectroscopy Facility (ETSF) and Nano bio Spectroscopy Group, Dpto. FÃsica de Materiales, Universidad Pais Vasco, Centro Mixto CSIC-UPV/EHU 20018 Donostia (Spain). http://nano-bio.ehu.es

²Institute for Electronics, Microelectronics, and Nanotechnology (IEMN), Lille, France

³Instituto Nazionale per la Fisica della Materia e Dipartimento di Fisica dell Universita di Roma Tor Vergata Via della Ricerca Scientifica, I-00133 Roma, Italy

We illustrate the effect of dimensionality and electron-hole attraction in boronnitride (BN) compounds. The optical absorption spectra of BN nanotubes are dominated by strongly bound excitons. The absolute position of the first excitonic peak is almost independent of the tube radius and system dimensionality. This provides an explanation for the observed optical gap constancy for different tubes and bulk hexagonal BN. Furthermore, the levels which are responsible for defectmediated photo-luminescence are shifted by the electric field making BN nanotubes excellent candidates for optoelectronic applications in the UV and below.

48

On the graphitisation role of oxide supports in carbon nanotube CVD synthesis

<u>Mark H. Ruemmeli</u>¹ Franziska Schaeffel¹ Christian Kramberger¹ Thomas Gemming¹ Paola Ayala¹ David Adebimpe¹ Bernd Rellinghaus¹ Ludwig Schultz¹ Bernd Buechner¹ Thomas Pichler¹

¹IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Systematic spectroscopic and microscopy studies on carbon nanotubes synthesized via chemical vapor deposition (CVD) using nano-engineered Fe particles on oxide supports were conducted. Our findings show that both the diameter and number of walls of the resultant CNT increase proportionally to the size of the catalyst particle. This behavior is fully consistent with catalyst volume to surface area constraints. In addition, detailed HREM studies on the carbon nanotubes show capped tops and open ended roots. The data points to the consecutive inward formation of concentric graphene caps during nucleation constricting and elongating the catalyst particle within the tube core. Further, the data suggest that after nucleation continued growth stems from the oxide support itself. This concept is further supported by CVD studies using graphite as the support and, in addition, studies on typical oxide supports alone show that such oxides can graphitize carbon species.

Understanding the Raman properties of graphite intercalated compounds: spectacular non-adiabatic effects, electron relaxation times and superconductivity

<u>A. Marco Saitta</u>¹ Matteo Calandra¹ Michele Lazzeri¹ Francesco Mauri¹ Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie, Paris

Graphite intercalated compounds (GIC's), intensely studied in the last 30 years, have recently gained a new large interest in the scientific community due to the discovery of a surprisingly high superconducting temperature in CaC₆. Moreover, GIC's are important in understanding the promising properties of intercalated nanotubes and doped graphene. Raman spectroscopy is an extremely powerful tool in characterising these materials, particularly through the analysis of the high-energy optical modes. However, the Raman-observed frequencies and linewidths show a large variability according to the system and of the intercalation level. We undertook a series of non-adiabatic ab initio calculations and adopted a theoretical scheme to directly relate the observed linewidths to the Drude electron relaxation time. We demonstrate that the puzzling experimental results can be fully understood in terms of our observed spectacular non-adiabatic effects. We show that the Raman linewidth-derived Drude relaxation times are a direct measure of the degree on non-adiabaticity and, in perspective, a powerful indicator of electron mobility and of potential superconducting properties. These results are shown to be general for layered metals, including MgB₂.

50

Properties of carbon nanotube composites aligned by self-organization

Giusy Scalia¹ Jan P. F. Lagerwall² Siegmar Roth¹

In our previous work we have demonstrated the alignment of carbon nanotubes (CNTs) via incorporation in self-organizing liquid crystalline (LC) matrices. This yields composites with macroscopic control of CNT orientation, exhibiting enhanced anisotropic optical, mechanical and electrical properties, as exemplified by our preparation of a composite highly loaded with well-dispersed SWCNTs that absorbs light strongly only for polarization parallel to the alignment direction, due to the aligned nanotubes. Our technique allows the use of any type of nanotube and can be combined with fractionation techniques for selecting only CNTs with a particular chirality, possibilities that we are currently exploring.

Moreover, a certain degree of CNT alignment is expected to improve electric per-

 $^{^1\}mathrm{Max}$ Planck Institute for Solid State Research, Heisenbergstrasse 1, 70176, Stuttgart

²Martin-Luther-University Halle-Wittenberg, Institute of Chemistry - Physical Chemistry, Muehlpforte 1, 06108 Halle/Saale, Germany

formance via a decreased percolation threshold. Our dielectric spectroscopy investigations of CNT - LC composites have shown percolation-like behavior along the alignment direction at very low CNT concentration, but essentially no conductivity in the perpendicular direction. We are now investigating the percolation threshold as a function of orientational order in our nanotube networks, simply employing the temperature dependence of the LC order. This makes it possible not only to continuously vary the degree of order but also to go from an organized to an isotropic state for the system.

51

Electrical detection of spin coherence in thin organic layers

<u>Sebastian Schaefer</u>¹ S. Saremi¹ K. Fostiropoulos² J. Behrends³ K. Lips³ W. Harneit¹

¹Fachbereich Physik, Freie Universitaet Berlin, Arnimallee14, 14195 Berlin, Germany

²Hahn-Meitner-Institut Berlin, Abteilung Heterogene Materialsysteme, Glienicker Str. 100, 14109 Berlin, Germany

³Hahn-Meitner-Institut Berlin, Abteilung Silizium-Photovoltaik, Kekule Str. 5, 12489 Berlin, Germany

An experimental demonstration of electrical detection of coherent spin motion of coupled spin-pairs in thin ZnPc films at room temperature is presented. Pulsed electrically detected magnetic resonance (pEDMR) experiments on vertical photocurrents through Al/ZnPc/ITO samples showed that an electron spin Rabi oscillation is recorded by transient current changes. The results are compared to similar experiments on C_{60} thin films that show weakly coupled spin-pairs [1]. Preliminary data indicate the presence of both weakly and strongly coupled pairs in ZnPc. Additional cw-EDMR-spectra and IV-curves as well as their sensitivity to different light intensities are discussed in the context of organic photovoltaic devices based on ZnPc and C_{60} .

1 W. Harneit, C. Boehme, S. Schaefer, K. Huebener, K. Fostiropoulos, and K. Lips, Phys. Rev. Lett. 98, 216601, (2007)

52

Carbon nanotube systems with highly anisotropic nanomagnets

<u>Franziska Schäffel</u>¹ Christoph Schünemann¹ Christine Täschner¹ Mark H. Rümmeli¹ Annett Gebert¹ Albrecht Leonhardt¹ Bernd Rellinghaus¹ Bernd Büchner¹ Thomas Pichler¹ Ludwig Schultz¹

¹IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

We present a comparative study on carbon nanotubes (CNT) grown from multilayer Fe-Pt thin films and predefined FePt nanoparticles via DC-plasma enhanced chemical vapour deposition (CVD) and thermal CVD, respectively. Fe-Pt multilayers are prepared in a DC-sputtering process. When subjected to the CVD process the thin films disintegrate into FePt islands of different sizes. In contrast, the predefined FePt nanoparticles can be controlled in terms of their size and areal density through the gas phase preparation process [1]. The plasma and thermal CVD conditions are tuned to obtain carbon nanotubes magnetically terminated with FePt nanoparticles, ideally in the $L1_0$ phase. The chemically ordered $L1_0$ phase of FePt exhibits a very high magnetic anisotropy which promotes significant interest in such nanoparticle-nanotube-systems for applications in magnetically actuated nanoelectromechanical systems.

1 F. Schäffel et al., Chem. Mater. 19, 5006 (2007).

53

Symmetry breaking in epitaxial graphene probed by ARPES

Aaron Bostwick¹ Jessica McChesney¹ Taisuke Ohta¹ K. V. Emtsev² <u>Th. Seyller</u>² Karsten Horn³ Eli Rotenberg¹

¹Advanced Light Source, Lawrence Berkeley National Lab, Berkeley

The energy bands of n-doped graphene on SiC(0001) have been observed to deviate significantly from the expected conical shape near the Dirac crossing [1]. Two scenarios have been proposed to explain these deviations, either as originated from the real part of the electronic self-energy due to many body interactions [1], or from A-B symmetry-breaking due to chemical interactions between the graphene and the underlying layer [2]. In this talk we present a number of arguments against the A-B symmetry breaking scenario, among which is the observed **k**-dependent intensity of the Fermi surface as measured by ARPES. We show that the observed intensity distribution is directly sensitive to the degree of A-B symmetry breaking and show that the upper limit for an energy gap in graphene on SiC is much smaller than the observed deviations in the band structure.

- 1 Bostwick et al. 2007, Zhou et al. 2007
- 2 Zhou et al.

54

Modeling of Graphene Field-Effect Transistor With a Step-Like and Barrier-Like Gate Potentials

<u>Alex Shevtsov</u>¹ Yuriy Klymenko² Sven Stafström³ Alexander Onipko⁴ National Taras Shevchenko University of Kyiv, 03022, Kyiv, Ukraine

²University of Erlangen

³Fritz Haber Institute

²Space Research Institute of National Academy of Sciences and National Space

Agency of Ukraine, 03187, Kyiv, Ukraine

³Department of Physics, IFM, Linköping University, S-581 83 Linköping, Sweden

Split-gate technique makes possible manufacturing junctions with a variable (ideally, in a step-like fashion) concentration of charge carriers along graphene ribbons and to control the width of the current channel. Such structures possess properties of a field effect transistor (FET) that can easily be understood within the modematching approximation: unit/zero transmission for coincident/different transverse quantum numbers of incident electrons and transmitted electrons or holes. In this approximation, ohmic current-gate voltage $(I(V_q))$ characteristic, as a function of $|eV_q - E_F|$, is represented by an ascending ladder, symmetric with respect to $V_g = E_F/e$, independently of whether the gate potential eV_g is step-like or barrierlike, and of the position of the Fermi energy E_F . The latter determines the maximal current which is attained in a ribbon with the given width at $|eV_q - E_F| = |E_F|$. This approximate picture is thoroughly elaborated by modeling the FET performance on the basis of the Landauer conductance formula with the exact account to the electronic structure of armchair and zigzag ribbons. The focus is put on how FET characteristics can be modified by exploiting the dependence of the channel conductance on the type (semi-metallic or semi-conducting), width, nature and concentration of current carriers, and ratio of the channel width to barrier thickness. We discuss associated links between two descriptions of gate-affected current in graphene ribbons: the Schrödinger (atomistic) and Dirac (continuous).

55

Confined catalytic reaction of organometallics inside carbon nanotubes

Hidetsugu Shiozawa

Advanced Technology Institute (ATI), University of Surrey, Guildford

Filled carbon nanotubes have aroused a rapidly growing interest as building blocks for nanotechnology. A large variation of host-guest pairs may provide for a new class of hybrid materials with novel electronic and magnetic properties. Here we show that the confined tubular space inside single-walled carbon nanotubes can act as a nanoreactor. As a model case we study the growth of inner shell tubes from encapsulated ferrocene and fullerene precursors. A combined spectroscopic and microscopic study unravels catalytic and non-catalytic routes to the inner tube growth. The confined catalytic process provides for the controlled growth of iron-based nanoparticles as well as the defined doping of tube materials. Hence, this work represents a new route for novel materials design.

⁴Bogolyubov Institute for Theoretical Physics, 03680, Kyiv, Ukraine

Optical Absorption in Ion-Irradiated Single Wall Carbon Nanotubes in the Far-Infrared Spectral Range

Viera Skakalova¹ Alan B. Kaiser² Siegmar Roth¹

 $^1\mathrm{Max}$ Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

²MacDiarmid Institute for Advanced Materials and Nanotechnology, SCPS, Victoria University of Wellington, P O Box 600, Wellington, New Zealand

The optical absorption of Ar^+ ion-irradiated and of $SOCl_2$ -doped single wall carbon nanotubes (SWNT) thin networks was measured and compared in the far-infrared and the visible spectral range. A surprising result is that absorption at low energies (<0.5 eV) increases both with Ar^+ irradiation and with $SOCl_2$ doping, this in spite of the fact that their electrical conductances behave differently. Upon irradiation, conductance decreases by orders of magnitude [1] while upon doping, conductance increased by a factor of 5 [2]. These results will be discussed in the frame of the Drude-Lorentz model used by Kampfrath et al. [3] involving indirect optical transitions assisted by phonon and defect scattering as well as on direct optical transitions in small-gap and metallic tubes.

- V. Skakalova, Y.-S. Woo, Z. Osvath, L. P. Biro, and S. Roth, *Phys. Stat. Sol. (b)* 243, 3346-3350 (2006)
- V. Skakalova, A. B. Kaiser, U. Dettlaff-Weglikowska, K. Hrncarikova and S. Roth, J. Phys. Chem. B 109, 7174-7181(2005)
- T. Kampfrath, L. Perfetti, F. Schapper, C. Frischkorn, and M. Wolf, Phys. Rev. Lett. 95, 187403 (2005)

57

Formation of a conductive nanotube network in polymer melts: Rheology and conductivity spectroscopy

Tetyana Skipa¹ Ango Alig¹ Dirk Lellinger¹ Petra Pötschke²

Destruction and formation of the conductive nanotube network in polymer melts has been investigated by a combination of conductivity spectroscopy and dynamic-mechanical analysis for polycarbonate containing multiwalled carbon nanotubes. The combined setup allows simultaneous time-resolved measurements of electric conductivity, dielectric permittivity and dynamic shear modulus. After annealing of the samples above glass transition a well defined, short shear deformation was applied to the melt. This deformation leads to a decrease of the conductivity by about seven orders of magnitude and of the real part of the shear modulus by a

¹Deutsches Kunststoff-Institut, Schlossgartenstr. 6, D-64289 Darmstadt, Germany ²Leibniz-Institut für Polymerforschung Dresden e.V. Hohestr. 6, D-01069 Dresden, Germany

factor of 20. In the rest time after the shear deformation a complete recovery of the conductivity and shear modulus was observed. Such a recovery of the electrical and mechanical properties of nanotube-polymer melts could be related to a process of aggregation of nanotubes in clusters and formation of a conductive network. For a quantitative description of the time-dependent electrical conductivity a model combining cluster aggregation and dynamic electrical percolation is applied.

58 Stability of carbon nanotubes to laser irradiation probed by Raman spectroscopy

<u>A. V. Soldatov</u>¹ D. Olevik¹ M. Dossot² V. Mamane³ B. Vigolo⁴ Y. Fort³ B. Humbert² E. McRae⁴

CNTs in a bundled state suffer from overheating effects - exposure to laser irradiation leads to a reversible shift of the RBM resonance window at a moderate laser fluence [1] or even to damaging of certain nanotube types at higher fluencies [2]. Here we report on our systematic study of the influence of laser irradiation on the Raman spectra of HiPCO-produced single wall CNTs. Specifically, we have examined Raman response of bundled CNTs to: i) laser power density; ii) exposure time and iii) photon energy (1.96 and 2.33 eV). Our results show that irreversible destruction of CNTs in the bundles takes place at even a moderate laser power density (500 W/cm2). Notably, the tubes with smaller diameters are influenced first and the rate of CNT damage increases with photon energy. Finally, we determined that the threshold for the RBM spectrum profile to change at about 200 W/cm2, which is apparently below the laser fluencies used typically in Raman experiments on CNT bundles. Based on these results we developed a regime of Raman data collection which was recently used to identify functionalization of different types of CNTs [3] from their RBM Raman spectra [4].

- 1 C. Fantini, et al. Phys. Rev. Lett., 93, 147406 (2004).
- 2 H. Huang, et al. J. Phys. Chem. B, 110, 7316, (2006).
- 3 J. Liu, et al. Carbon, 45, 885, (2007).
- 4 J. Liu, et al. Physics E, in press.

¹Department of Applied Physics and Mechanical Engineering, LuleåUniversity of Technology, SE - 971 87, Luleå, Sweden

²Laboratoire de Chimie Physique et Microbiologie pour l

³Laboratoire de Synthese Organometallique et Reactivite, Nancy Universite, Nancy Universite, UMR 7565 CNRS, 54506 Vandoeuvre les Nancy cedex, France

⁴Laboratoire de Chimie du Solide Mineral, Nancy Universite, UMR 7555 CNRS, 54506 Vandoeuvre les Nancy cedex, France

Oxidation induced defects in CVD grown carbon nanotubes for peapod synthesis

 $\frac{\text{Christian Spudat}^1}{^1\text{Research Centre}}$ Carola Meyer 1 Christian Kramberger 2 Claus Michael Schneider 1 Research Centre Juelich, Institute for Solid State Research, Electronic Properties, 52425 Juelich

²Institute for Solid State and Materials Research (IFW) Dresden, 01171 Dresden

Carbon nanotubes (CNTs) filled with C₆₀ Fullerenes, so-called "peapods", form a model system for studying one-dimensional molecular chains coupled to a ballistic conductor. In general, these peapods are synthesized by filling "bulk' material, and they are successively dispersed on a substrate from solution. The disadvantage of this method is that the nanotubes are rather short due to prior sonication and bundle together in ropes. Thus, characterization of single peapods is rather difficult. Because of that, the CTNs are grown directly on substrates by using the CVD method. To fill them, it is necessary to open the carbon nanotubes without causing too much damage for later transport measurements. Therefore, a characterization of oxidation induced defects in carbon nanotubes is needed finding the right parameters for opening without destroying the nanotubes completely. This has been done for bulk-material arc discharge nanotubes but the procedure is not the same for individual CVD nanotubes grown on substrate. In general two different opening methods are used: Oxidation by acid treatment and heat treatment in air. We investingate the effects of these two methods on CNTs correlating AFM, HR-TEM and FT-Raman spectroscopy. Characterization of defects in CNTs is often done using the ratio of G-mode and D mode Raman spectroscopy. But the intensity of the D-peak is also sensitive to amorphous carbon, which sits at the outer walls of the nanotubes. Using FT-Raman for characterization, we could observe a shift of the G-peak in Raman spectra during the oxidation process, which has not been investigated in this respect, so far.

60

Franck-Condon blockade in suspended carbon nanotubes

<u>Christoph Stampfer</u>¹ Renaud Leturcq¹ Kevin Inderbitzin¹ Lukas Durrer² Christofer Hierold² Klaus Ensslin¹

Carbon nanotubes, which can be thought of either as one-dimensional solids or macromolecules, are prominent candidates to study interactions of charge carriers with (discrete) molecular vibrational modes. Here, we report on the Franck-Condon blockade in a quantum dot formed in a suspended single-walled carbon nanotube (SWNT) device [1]. The suspended SWNT quantum dot is sandwiched between a back-gate and a freestanding top gate, providing a large tunability of the electronic

¹Nanophysics, ETH Zurich, 8093 Zurich, Switzerland

²Micro and Nanosystems, ETH Zurich, 8092 Zurich, Switzerland

properties. The fourfold degeneracy of the SWNT quantum dot energy spectrum is evident in Coulomb diamond measurements at 1.3K showing the high quality of the device. For the electronic excited states we find a typical energy of 5 meV. In addition we observe excited states with energy spacings of 0.5-0.9 meV, which we attribute to longitudinal phonons in the clamped nanotube device. The exponential suppression of the sequential-tunneling current at low bias is a clear signature of Franck-Condon blockade with very strong electron-phonon coupling.

1 C. Stampfer, A. Jungen, R. Linderman, D. Obergfell, S. Roth, and C. Hierold, Nano Lett., 6 (7), 1449-1453, (2006).

61

Potential Barriers in Graphene

<u>Nimrod Stander</u>¹ Benjamin Huard¹ Joey Sulpizio¹ Kathryn Todd¹ David Goldhaber-Gordon¹

¹Stanford University, Stanford

Graphene, a single layer of graphite, is a gapless semiconductor, with carriers that should behave as massless Dirac fermions. One of the striking predicted phenomenon in clean graphene is the full transmission (with probability one) of its charge carriers, when crossing perpendicularly through a potential barrier, at any energy. This phenomenon, reminiscent of the Klein paradox for spin 1/2 relativistic particles, can be probed via the transport properties of charges in a sheet of graphene with well-chosen potential profiles imposed by top gates. Idealized predictions for transmission across potential barriers may be modified by the presence of disorder (Coulomb impurities close to the graphene sheet) combined with the unusual screening properties of graphene. I will present transport measurement on samples where the graphene sheet is gated both globally by a back gate, and locally by a top gate, allowing the creation of various potential configurations. Measuring many such samples with varying top gate lengths and top gate dielectric thicknesses, we show that in the majority of our devices, and for most accessible densities, transport across the barrier is diffusive. However, for some of our highest mobility devices, with carrier densities as high as 10^{13} cm⁻², the graphene is expected to be in the ballistic regime. The experimental results indeed deviate from those calculated by the diffusive model, which might indicate that ballistic effects are becoming important.

62

Single-wall carbon nanotubes as DNA-delivery vector

C.Y. Li¹ F.H. Lin² C.K. Hsu¹ L. Stobinski³

¹Department of Material Science and Engineering, National Taipei University of Technology, Taipei, Taiwan

²Department of Biomedical Engineering, National Taiwan University, Taipei, Tai-

wan

³Institute of Physical Chemistry, Polish Academy of Sciences, Poland, lstob@ichf.edu.pl

Preparation of a new, stable gene carrier would be of great practical importance to improve the transfection efficiency in gene therapy, such as therapeutic protein formation, immunogenicity enhancement and apoptosis induction. The stability and applicability of the system containing single-walled carbon nanotubes (SWCNTs) in combination with certain sequence of plasmid DNA (EGFp-C1) were also examined by computer simulation. Raman spectroscopy was used to verify the SWCNT-DNA complex formation. Diamine molecules (putrescine and polyoxyethylene-bis-amine) were used to create positive charge on the SWCNT surface (similarly to physiological conditions) and also enhance the binding ability of EGFp-C1 to CNT. The formation of peptide bond was examined by FTIR to confirm the crossliking process. The amount of surface functional groups was tested by TGA method. Biocompatibility was evaluated with LDH, MTT and total DNA. The results demonstrate increase in cell viability and the presence of SWCNT-putrescine complex. IL-6 release was measured to justify the inflammatory induction. The binding efficiency of functionalized SWCNTs to EGFp-C1 was also analyzed by electrophoresis to demonstrate their binding strength. Tests in-vitro showed that transfection was not significantly higher than other non-viral vectors. It could be due to quite high stability of SWCNT-DNA complexes.

63

MoSIx connectivity in self-assembled networks

<u>Jure Strle</u>¹ Damjan Vengust¹ Mihaela Ploscaru¹ Marko Uplaznik¹ Dragan Mihailovic¹

¹Department of Complex Matter, Jozef Stefan Institute, Ljubljana, Slovenia

Inorganic $Mo_6S_{9-x}I_x$ (MoSIx) molecular nanowires have recently been shown to easily bond to gold nanoparticles (GNPs) due to their sulfur terminated ends, which potentially opens the way to self-assembly of large electronic circuits in molecular electronics.

We report an AFM investigation on the properties of irregular self-assembled MoSI - 5 nm diameter GNP networks made in solution and deposited on different substrates. The networks are typically on a scale of up to several tens of micrometers, but also much larger ones have been observed, extending over 1000 square microns. The connectivity properties of one such network have been analyzed in more detail by statistically measuring the heights of particles and nanowires, as well as the number and the angle of attachment of the nanowires connected at the vortices.

We have also monitored the network stability with time in ambient conditions by repeatedly measuring its topographic picture over a period of eight months. Although the network survives intact over this period, some degradation has been observed. Specifically, the nanoparticles have been reduced in size and nanowire diameter has also decreased.

The experiments show that the MoSI-GNP system exhibits specific connectivity patterns, which may be used to design and construct connections in molecular-scale electronic networks.

64

Widely Tunable Laser Mode-Locked by Single-wall Carbon Nanotubes

F. Wang¹ V. Scardaci¹ Z. Sun¹ A. G. Rozhin¹ I. H. White¹ A. C. Ferrari¹ Engineering Department, University of Cambridge, Cambridge, UK

Ultrafast optical pulse sources with spectral tuning capabilities have widespread applications in laser spectroscopy, laser photochemistry, biomedical research and telecommunications. One approach to realize such sources is to directly apply a wavelength-tuning element inside a mode-locked laser cavity. However, to enable wide-tuning, it is necessary to use a saturable absorber with a large operating bandwidth, preferably larger than the gain bandwidth of the active medium. Single Wall Carbon nanotubes (SWNT) have been successfully used to generate sub picosecond laser pulses in a broad spectral range between 1.04 and 1.6 microns [1-3]. By controlling the SWNT diameter distribution during growth it is possible to tune the absorption maximum and bandwidth in a desired range. Here we report a novel SWNT- polycarbonate polymer composite, with an absorption maximum at 1550 nm and a bandwidth of about 300 nm [3,4]. The composite shows strong saturable absorption with saturation intensity of 7 MW/cm². We also demonstrate the first SWNT-mode-locked widely tunable fibre ring laser [5]. This is achieved through the control of amplification at the specific transitions of the Er³⁺ gain medium by placing a band-pass filter in a laser cavity. The laser generates 2.4 ps pulses continuously tunable between 1518 and 1558 nm with average power of 0.3 mW [5]. Besides the wide tuning range, this laser also features a high optical signal-to-noise ratio and an excellent jitter performance. A working laser will be demonstrated at the conference.

- 1 G. Della Valle et al., Appl. Phys. Lett. 89, 231115 (2006).
- 2 A. G. Rozhin et al. Physica Status Solidi B, 243 3551 (2006).
- 3 A. G. Rozhin et al. submitted (2008).
- 4 V. Scardaci et al. submitted (2008).
- 5 F. Wang et al. submitted (2008).

Longitudinal optical phonons in metallic and semiconducting carbon nanotubes

 $\underline{\underline{Hagen~Telg}^1}$ Martin Fouquet 1 Janina Maultzsch 1 Yang Wu 2 Bhupesh Chandra 3 J. \underline{Hone}^3 Tony F. Heinz 2 C. Thomsen 1

¹Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

²Departments of Electrical Engineering and Physics, and Nanoscale Science and Engineering Center, Columbia University, New York 10027, USA

³Department of Mechanical Engineering, and Nanoscale Science and Engineering Center, Columbia University, New York 10027, USA

We analyze the high-energy Raman modes, G^+ and G^- , in a pair of one metallic and one semiconducting nanotube grown across a $100\,\mu\mathrm{m}$ wide slit. By combining Rayleigh scattering with Raman resonance profiles of the radial breathing mode and the high-energy modes, we assign the broad G^- peak to a metallic and the G^+ peak to a semiconducting nanotube. Considering theoretical predictions we show that both peaks, G^- and G^+ , originate from the LO phonon. The G^- peak is the longitudinal mode of the metallic tube; it is broadened and downshifted due to strong electron-phonon coupling in the metallic nanotube. The G^+ peak is due to the longitudinal mode in the semiconducting tube. We conclude that the presence of the G^+ peak at 1590 cm $^{-1}$ in an assumed single isolated metallic nanotube in fact originates from an additional semiconducting nanotube.

66

Infrared spectroscopy on the fullerene C₇₀ under pressure

 $\underline{\text{Komalavalli Thirunavukkuarasu}^1}$ Christine Kuntscher 1 Ferenc Borondics 2 Gyöngyi Klupp 2 Katalin Kamar 2

¹Chair of Experimental Physics II, University of Augsburg, D-86153 Augsburg, Germany

²Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O.Box 49, Budapest, Hungary H 1525

 C_{70} is the most commonly occurring higher order fullerene next to C_{60} . Although several experimental investigations have been performed on this compound, the properties of C_{70} are not yet well understood. On cooling, C_{70} undergoes two orientational ordering transitions, one at 350 K and the other at 280 K, which are accompanied by structural phase change [1]. The pressure-induced orientational ordering in C_{70} is expected at around 1 GPa [2]. An earlier pressure-dependent infrared study on pure C_{70} could identify only eleven vibrational modes and found no discontinuous change in their pressure-dependence [3]. More detailed investigations are therefore necessary to find clear signatures of possible orientational ordering transitions and other pressure-induced phenomena in C_{70} under pressure.

We carried out pressure-dependent transmittance measurements on the C_{70} compound over a broad frequency range (400-22000 cm⁻¹) for pressures up to 10 GPa. Most of the vibrational modes were observable up to the highest measured pressure. They exhibit an anomaly in their pressure-induced frequency shift at around 0.7 GPa. The shift of the electronic absorption edge with increasing pressure is presented and discussed as well.

Supported by the DFG.

- 1 G. B. Vaughan et al., Chem. Phys. 178, 599 (1993).
- 2 H. Kawamura et al., J. Phys. Chem. Solids **54**, 1675 (1993).
- 3 H. Yamawaki et al., J. Phys. Chem. 97, 11161 (1993).

67

Raman spectroscopy study of nanobud structure on a freestanding individual carbon nanotube

<u>Ying Tian</u>¹ Delphine Chassaing¹ Albert G. Nasibulin¹ Paola Ayala¹ Hua Jiang¹ Anton S. Anisimov¹ Esko I. Kauppinen¹

¹NanoMaterials Group, Laboratory of Physics and Center for New Materials, Helsinki University of Technology, P.O. Box 5100, 02150 Espoo, Finland

Fullerenes and carbon nanotubes (CNTs) have attracted great interest from both fundamental and applied points of view due to their remarkable physical and chemical properties. Recently, we have reported a new hybrid material, Nanobuds, in which the fullerenes are covalently bonded to the outer surface of single-walled carbon nanotubes (SWCNTs). The experimental method used for continuous synthesis of Nanobuds is based on ferrocene vapor decomposition in a CO atmosphere, and the key parameter is the presence of trace concentrations of H2O vapor and CO2 acting as etching agents.

Combining with the transmission electron microscopy (TEM) experiment, we present for the first time the Raman spectroscopy study of the Nanobuds structure on a freestanding SWCNT. Both the characteristic features of SWCNT and fullerenes were observed in the Raman spectrum simultaneously using a 2.32eV excitation. The G-line and the radial breathing mode (RBM), which are well known to be a fingerprint of SWCNTs were identified, as well as the fullerenes characteristics signal. We present the evidence of Nanobuds on a 1.84nm nanotube with (16, 11) assigned chirality. The electron diffraction analysis on the same freestanding SWCNT results give the same chirality (16, 11). Besides the features from SWCNT, another weaker but clear band is observed around 1465cm-1, and this is associated with the typical vibrational modes of fullerenes, which confirm the nanobuds structure on the SWCNT.

Optical and magnetic properties of Er-doped fullerenes for quantum computation

<u>Archana Tiwari</u>¹ Geraldine Dantelle¹ John J. L. Morton² Kyriakos Porfyrakis¹ Andrew A. R. Watt¹ Arzhang Ardavan² G. Andrew D. Briggs¹

¹QIP IRC, Department of Materials, University Of Oxford, Oxford OX1 3PH, UK ²Clarendon Laboratory, Department of Physics, University Of Oxford, Oxford OX1 3PU, UK

Endohedral fullerenes are promising materials for quantum computation using electron spins that arise from the endohedral atom or atomic cluster to store or interact quantum information. We will discuss the optical control of endohedral spin and examine its potential as a readout mechanism for quantum computing schemes. We report the detailed characterization of several erbium doped fullerenes, in particular ${\rm ErSc_2N@C_{80}}$. Our study demonstrates that ${\rm ErSc_2N@C_{80}}$ has strong photolumine-scence (PL) at 1.5 $\mu{\rm m}$ as well as EPR activity from the ${\rm Er^{3+}}$ ion which can be driven optically. Er-doped fullerenes have been purified under HPLC and are characterized by absorption, PL and magnetic spectroscopy using EPR and SQUID. These characterizations give us a detailed insight into the electronic structure of ${\rm Er^{3+}}$ inside the cage arising from the crystal-field effect and external magnetic field perturbations. The direct optical access to ${\rm Er^{3+}}$ states without interrupting ${\rm C_{80}}$ cage may allow us to probe, address and manipulate the spin states which encode quantum information.

69

Non-covalent spin labeling of carbon nanotubes

S. Toth¹ D. Quintavalle¹ B. Nafradi² L. Forró² L. Korecz³ F. Simon¹

¹Institute of Physics, Budapest University of Technology and Economics, Budapest Hungary

²Institut de Physique de la Matiere Complexe, EPFL, CH-1015 Lausanne Switzerland

³Chemical Research Center of the Hungarian Academy of Sciences, Budapest Hungary

Non-covalent spin labeling of carbon nanotubes is presented. We fill inside SW-CNTs TEMPO (2,2,6,6-Tetramethylpiperidine-1-oxyl) molecules and study the rotational properties and thermal stability using electron spin resonance (ESR). We find that its rotation is hindered and non-isotropic. We also studied the thermal stability and the spin-lattice relaxation of N@ C_{60} peapod system. We find that the N escapes at higher temperatures for the encapsulated material as compared to its pristine, crystalline form. The temperature dependent spin-lattice relaxation time, T_1 , of the encapsulated molecule is significantly shorter than that of the crystalline material, which is explained by a charger transfer between the nanotubes and the

fullerenes.

70

Raman Study of Photosystem I and II and its Pigment beta-Carotene

<u>N. Tschirner</u>¹ K. Brose¹ M. Schenderlein² A. Zouni² P. Hildebrandt² C. Thomsen¹ Institut für Festkörperphysik, TU Berlin

Due to their ability to absorb light energy photosystem I and II are the most important protein complexes enabling photosynthesis in higher plants. Both photosystems contain different types of photoactive pigment molecules, one of the most important is carotene, which in addition to its light absorbing ability also serves a protective function within the protein.

Raman spectra of Photosystem I and II excited in the Soret region are presented and compared with resonance Raman spectra of β -carotene. Main focus is the vibrational band ν_1 around 1500 cm⁻¹, which originates from the ground-state inphase double bond C=C stretching mode of the isoprene units forming the backbone of β -carotene. The band consists of two unresolvable peaks possessing different resonance excitation profiles leading to a wavelength dependent shift of the band. Theoretical approaches trying to explain this behavior are discussed like different Frank-Condon enhancement of the two modes due to different excited-state displacements of the vibrational modes or Duschinsky rotation, which describes intensity changes of resonance excitation profiles due to mode mixing.

71

Electron transport and hot-phonon generation in carbon nanotubes

Niels Vandecasteele¹ Michele Lazzeri¹ Francesco Mauri¹ IMPMC, Pierre et Marie Curie, Paris

Metallic carbon nanotubes can carry the highest current density before they break. This makes them the best candidates as interconnects in future electronic devices. For voltages > 0.2 V, the measured IV curve of metallic tubes displays a sudden increase of the resistivity which is due to the scattering with optical phonons. Recently, we have shown [1] that the largest part of this electrical resisitivity is due to the presence of an anomalously-high optical-phonon occupation (hot phonons). Basically, during transport, the conducting electrons scatter with optical phonons. If the rate at which optical phonons are generated is faster than the rate at which they can release energy to the system, their population increases. This hot-phonon generation, in turn, augments the electrical resistivity of the system. Here, we will show how it is possible in practice to diminish the hot-phonon population and, thus, to improve the electrical performances of metallic tubes.

1 Lazzeri et.al. Phys.Rev.Lett. **95**, 236802 (2005)

²Institut für Physikalische Chemie, TU Berlin

2 Lazzeri et.al. Phys.Rev.B **73**, 165419 (2006).

72

Visualizing Electronic Properties of Carbon Nanotube Devices by Voltage Contrast Scanning Electron Microscopy

Aravind Vijayaraghavan¹ Sabine Blatt¹ Ralph Krupke¹

 $\overline{\mbox{ }^{1}}$ Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany

The most common technique to observe Single-Walled Carbon Nanotubes (SW-CNTs) is Scanning Electron Microscopy (SEM). However, this is limited to locating the nanotube, and is unable to provide structural or electronic information. We present Voltage Contrast SEM (VC-SEM) as a powerful technique for electronic characterization of high-density arrays of SWCNT devices [1] and to visualize the voltage-profile and charge-distribution in a single nanotube.

The most significant result is to distinguish between metallic and semiconducting SWCNTs in a SEM. This is achieved by observing the difference in contrast profile arising from charge-distribution when the nanotube is subjected to an asymmetric electric field. The observed charge-distribution will be explained through numerical simulations of the band-structure [2] under the influence of an asymmetric gate-field generated by our electrode configuration.

VC-SEM is many orders of magnitude quicker in comparison to Kelvin force or near-field microscopy. It can simultaneously characterize a high-density array of devices and sort them into metallic and semiconducting varieties and give an indication of the turn-on voltage required for the nanotube devices.

- 1 Vijayaraghavan, A., et al., Ultra-Large Scale Directed Assembly of Single-Walled Carbon Nanotube Devices. Nano Letters, 2007, 7(6).
- 2 Blatt, S., et al., Electrostatic Modeling of Carbon Nanotube Field Effect Transistors. IWEPNM 2008.

73

New method for single wall carbon nanotubes growth based on channel spark ablation

 $\underline{\text{Viliam Vretenar}}^1$ Petr Nozar^2 Carlo Taliani 3

The present contribution deals with a novel method for low-cost single wall carbon nanotubes (SWCNT) production. This method represents a synthesis of methods

¹Danubia NanoTech, sro, Ilkovicova 3, 812 19 Bratislava, Slovakia

²Istituto per lo Studio dei Materiali Nanostrutturati (ISMN), CNR, Via P. Gobetti, 101, 40129 Bologna, Italy

³Organic Spintronics, Srl, Via P. Gobetti, 101, 40129 Bologna, Italy

based on both a production of catalyst nano-particles by plasma heating and a decomposition of carbon enriched gas by CVD ones. Even if the experiments are highly tentative and development of apparatus is still in progress, the results are very promising. All experiments were carried out in argon atmosphere with methane admixture, using standard NiCo catalyst. Besides fine Raman spectra of samples produced by reported procedure, very narrow distribution of SWCNTs diameters has been observed by optical absorption spectroscopy. Moreover, TEM pictures indicate that SWCNTs are isolated and not tied into bundles. On the other hand, thermo-gravimetric analysis has revealed huge amount of metal particles inside the samples. Surprisingly, introduction of stainless steel catalyst instead of harmful and expensive NiCo, has led to same results.

74

Dynamics of paramagnetic metallofullerenes in peapods

Takao Akachi¹ Haruya Okimoto¹ Yasuhiro Ito¹ Hisanori Shinohara¹ <u>Jamie H Warner</u>² Andrew A. R. Watt² Mujtaba H. Zaka² Kyriakos Porfyrakis² Ling Ge² G. Andrew D. Briggs² Arzhang Ardavan³

The metallofullerenes (MFs), (Sc@C82 and La@C82) have excellent electron spin properties due to the unpaired electron transferred from the metal atom to the carbon cage. These materials hold great promise for quantum information processing using electron spin qubits. One-dimensional chains of spin are formed by inserting the MFs into single-walled carbon nanotubes.

In this work, we reveal insights into the unique behaviour of MFs in peapods using low-voltage TEM. By using electrons accelerated at 80kV in TEM we minimize damage to the carbon structures and monitor the MFs for extended periods. We observe oscillations of single, coupled and groups of MFs along the axis of the nanotube. The time-dependent rotational dynamics of La@C82 and Sc@C82 are examined and distinct differences in their behaviour is observed. We observe elastic breathing-like radial expansion and contraction of individual isolated SWNT peapods. The expansion leads to changes in the 1D packing of the MFs. This expansion is driven by energy transfer from electron beam irradiation to the MFs. The dynamic motion of MFs in peapods is demonstrated with time-series of TEM images and compiled movies.

¹Department of Chemistry and Institute for Advanced Research, Nagoya University, Nagoya

²Department of Materials, University of Oxford, Oxford

³Department of Physics, University of Oxford, Oxford

Molecular systems: optical switching measurements by indirect coupling and induced superconductivity by direct coupling experiments

 $\underline{C.B.~Winkelmann}^1$ N. Roch 1 I. Ionica 1 X. Chevalier 2 C. Bucher 2 G. Royal 2 W. Wernsdorfer 1 F. Balestro 1 V. Bouchiat 1

¹Institut Neel - CNRS/UJF Grenoble France

 $^2\mathrm{DCM}$ / UJF Grenoble France

We study porphyrin derivative coated silicon nanowire field effect transistors (SiNW-FETs), which display a large, stable, and reproducible conductance increase upon illumination (1). The efficiency and the kinetics of the optical switching are studied as a function of gate voltage, illumination wavelength, and temperature. The decay kinetics from the high- to the low-conductance state is governed by charge recombination via tunneling, with a rate depending on the state of the SiNW-FET. The comparison to porphyrin-sensitized carbon nanotube FETs allows the environment- and molecule-dependent photoconversion process to be distinguished from the charge-to-current transducing effect of the semiconducting channel. In parallel, we will briefly present first measurements on superconducting transport

In parallel, we will briefly present first measurements on superconducting transport through a single fullerene molecule. Nanometric junctions are fabricated by the electromigration technique. Gate effects are induced by an Al / Al₂O₃ backgate. Using the superconducting proximity effect, the nano-junctions without molecules show a well defined Josephson current, and Andreev reflections are also observed. Preliminary results on the effect of superconductive electrodes on a single C_{60} molecule down to 50 mK are presented.

(1) C.B. Winkelmann et al., Nano Lett. 7, 1454 (2007).

In-situ catalyst screening for carbon nanotube growth

Stephan Hofmann¹ Raoul Blume² <u>Christoph Tobias Wirth</u>¹ Mirco Cantoro³ Renu Sharma⁴ Caterina Ducati⁵ Michael <u>Haevecker</u>² Spiros Zafeiratos² Peter Schnoerch² Andreas Oesterreich² Detre <u>Teschner</u>² Martin Albrecht⁶ Axel Knob-Gericke² Robert Schloegl² John Robertson¹

¹Department of Engineering, University of Cambridge, Cambridge

²Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

³IMEC, AMPS/NANO,3001 Leuven, Belgium

⁴LeRoy Eyring Center for Solid State Science, Arizona State University, Tempe AZ85287-1704, USA

 $^5\mathrm{Department}$ of Materials Science and Metallurgy, University of Cambridge, Cambridge CB2 3QZ, UK

⁶Institut fuer Kristallzuechtung, Max Born-Str. 2, D-12489 Berlin, Germany

A detailed understanding of the processes involved in the catalytic chemical vapour deposition (CVD) of carbon nanotubes is important to achieve the desired degree of growth control. We present a systematic study of catalyst-support and catalyst-carbon interactions during SWNT growth by combining environmental transmission microscopy (ETEM) and in-situ, time-resolved X-ray photoelectron spectroscopy (XPS) [1]. We focus on Ni, Fe, Pd and Au model catalyst films on SiO2 during pre-annealing in O2 and NH3 and during C2H2 decomposition. At the conditions used all metal films dewetted into nm-sized crystals, whereby only Ni and Fe catalysed SWNTs. A SWNT nucleates by lift-off of a carbon cap. Cap stabilization and nanotube growth involve the dynamic reshaping of the catalyst nano-crystal itself [2]. Pd and Au are less efficient in dissociating C2H2 and C is more weakly bound to their surfaces. Deliberately oxidised Fe gave no SWNT growth, which allowed a clear assignment of the catalytic pathway of carbon nanotube formation.

- 1 Hofmann S., Blume R., Wirth C. T., et al. to be published (2008).
- 2 Hofmann S., Sharma R., Ducati C., Du G., Mattevi C., Cepek C., Cantoro M., Pisana S., Parvez A., Ferrari A. C., Dunin-Borkowski R., Lizzit S., Petaccia L., Goldoni A., Robertson J., Nano Lett. 7, 602 (2007).

Metal Catalyst in CVD Growth of Carbon Nanotubes: Role of Chemical Composition

Oleg V. Yazyev^{1,2} Alfredo Pasquarello^{1,2}

¹Ecole Polytechnique Fédérale de Lausanne (EPFL), Institute of Theoretical Physics (ITP), CH-1015 Lausanne, Switzerland

²Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), CH-1015 Lausanne, Switzerland

The inability of performing growth of carbon nanotubes (CNTs) with predetermined chirality indices and thus electronic properties is the major obstacle on the way to incorporating CNTs into electronic devices. The chemical vapor deposition (CVD) growth of CNTs catalyzed by metallic nanoparticles is believed to be the most promising approach for reaching this goal. For a long time, the catalyst composition has been limited to iron-group metals. However, it has recently been shown that metallic nanoparticles of many other metals, including inert coinage metals, are also able to act as catalysts in the CVD growth process. This calls for a comprehensive study of the role of the metal catalyst chemical composition to achieve optimal growth conditions and enhance the preference for definite chiralities.

Here, we model the crucial steps of CVD growth of CNTs from first principles by considering late transition (Ni, Pd, Pt) and coinage (Cu, Ag, Au) metal catalysts. For all metals, we considered various diffusion mechanisms including both surface and subsurface channels, finding the lowest activation barriers for carbon adatoms on nanoparticles of coinage metals. For these metals, our calculations further show that the diffusion is restricted to the nanoparticle surface when diatomic carbon is initially obtained from the decomposition of the precursor gas. From the binding energies of armchair and zigzag edges of CNT fragments, we infer a high preference for the growth of armchair CNTs on Cu nanoparticles. These results indicate that coinage metal catalysts favor CVD growth of CNTs at low temperatures and with narrow chirality distributions.

78

Magnetic carbon nanostructures for spintronics and quantum computing: first principles studies

Oleg V. Yazyev^{1,2}

¹Ecole Polytechnique Fédérale de Lausanne (EPFL), Institute of Theoretical Physics (ITP), CH-1015 Lausanne, Switzerland

²Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), CH-1015 Lausanne, Switzerland

Magnetic materials and nanostructures based on carbon and other light elements provide a number of attractive opportunities for future information technologies such as spintronics and quantum information processing. This novel field of carbon-

based magnetism has attracted considerable attention due to the recent experimental observations of ferromagnetism in graphitic materials. I review the results of theoretical studies of the magnetism induced by point defects [1] and edges in graphene and related nanostructures. Particular attention is devoted to the question of long-range magnetic order at one-dimensional zig-zag graphene edges [2] considered as a basis for novel spintronics devices. I also discuss hyperfine interactions, the magnetic interactions between the spins of electron and nuclei, in graphenic carbon nanostructures [3]. Some recipes for achieving maximum electron spin decoherence times in graphene-based nanostructures are given.

- O. V. Yazyev and L. Helm, Phys. Rev. B 75, 125408 (2007).
- O. V. Yazyev and M. I. Katsnelson, Phys. Rev. Lett., in press [arXiv:0711.0207].
- O. V. Yazyev, arXiv:cond-mat/0702424.

79

Controlling metallofullerene spin-spin interactions in diluted fullerene solids.

Mujtaba H. Zaka¹ Jamie H. Warner¹ Andrew A. R. Watt¹ Kyriakos Porfyrakis¹ Takao Akachi² Haruya Okimoto² Yasuhiro Ito² Arzhang Ardavan³ Hisanori Shinohara² G. Andrew D. Briggs¹

Metallofullerenes are encapsulated metal atoms inside a hollow fullerene cage. They possess many unique properties, compared to empty fullerenes, due to the transfer of electrons from the metal atom to the fullerene cage. The spin of the unpaired electron on the C82 cage of either Sc@C82 or La@C82 metallofullerenes is very interesting and important for quantum information processing. For this reason, further understanding of the dynamics of spin-spin interactions between metallofullerenes in a solid matrix is required.

The spin-active metallofullerenes Sc@C82 and La@C82 are diluted quantitatively with C60. This enables control over the average inter-fullerene distance and this changes the spin-spin interactions between metallofullerenes. Electron spin resonance is used to probe the concentration dependent dynamics of the systems. Results indicate increased signal structure with increased dilution. The metallofullerene systems have been modeled to further understand the nature of the spin-spin interactions. These encouraging results provide a platform for further research into using peapods structures for quantum information processing.

¹Department of Materials, University of Oxford

²Department of Chemistry, Nagoya University

³Department of Physics, University of Oxford

Novel carbon nanotube network deposition technique for fabricating electronic devices

<u>Marina Y. Zavodchikova</u>¹ Albert G. Nasibulin¹ Kestutis Grigoras² Tero Kulmala² Sami Franssila² Vladimir Ermolov³ Esko I. Kauppinen¹

¹NanoMaterials Group, Laboratory of Physics and Center for New Materials, Helsinki University of Technology, Espoo, Finland

²Microfabrication Group, Micro and Nanosciences Laboratory, Helsinki University of Technology, Espoo, Finland

³Nokia Research Center, Helsinki, Finland

Carbon nanotube networks (CNTNs) are found to be a promising material for electronic applications. An attractive feature of CNTNs is that they retain many of the interesting electronic properties of individual SWCNTs while providing the processing capabilities of mass fabrication methods. Nowadays there are multiple wet techniques of CNTN deposition from a surfactant solution, used in thin-film transistor fabrication, available. We present a novel efficient dry deposition process of random SWCNTNs of various controllable densities onto a substrate directly from the gas phase at ambient pressure and room temperature. SWCNTs were produced by thermal decomposition of ferrocene in the presence of CO in a vertical laminar flow reactor [1]. Due to spontaneous charging of SWCNTs during their synthesis [2], an electric field, which guides the nanotubes towards the substrate surface, was employed for the efficient deposition. In order to collect nanotubes from the gas flow downstream of the reactor and deposit them directly on to the substrate, we applied a homogeneous electric field using an electrostatic precipitator [3]. This allows SWCNTs to be directly deposited in patterned or homogeneous films on substrates at room temperature immediately after synthesis. While solution-based SWCNT deposition may alter the nanotube pristine properties, our direct dry deposition technique gives a possibility to obtain networks of high purity and quality SWCNTs. Presented technique was applied for the fabrication of SWCNTN-based field-effect transistors (FETs). Lower density photolithographically patterned SWCNTNs exhibited p-type semiconducting thin film behavior. Electrical measurement results of as-produced SWCNTN-based FETs will be demonstrated.

- 1 A.Moisala, A.G.Nasibulin, S.D.Shandakov, H.Jiang and E.I.Kauppinen, Carbon 43 (2005) 2066-2074
- 2 D.Gonzalez, A.G.Nasibulin, S.D.Shandakov, H.Jiang, P.Queipo and E.I.Kauppinen, Carbon 44 (2006) 2089-2108
- 3 T.J.Krinke, K.Deppert, M.H.Magnusson, F.Schmidt and H. Fissan, Aerosol Science 33 (2002) 1341-1359

81 Growth of Carbon Nanotubes towards applications as horizontal Interconnects

 $\underline{\text{Can Zhang}}^1$ Daire Cott^2 Nicolo Chiodarelli 2 Philippe Vereecken 2 John Robertson 1 Caroline Whelan 2

We evaluate the possibility of achieving horizontal carbon nanotube (CNT) interconnect structures. Firstly, CNT forests are grown on planar conducting substrates, including 500 nm poly-Si and 15 nm TiN/TaN, using NH3 plasma annealed Co/Ni PVD deposited thin film catalysts using C2H2 or C2H4 as carbon source in thermal CVD as low as 500-600 °C. In order to achieve similar yield of CNTs from a vertical surface, horizontal growth test structures (HGTS) were fabricated by Intel Ireland. These structures comprise of 200 nm high vertical poly-Si (poly-Si HGTS) or CoSi2 (CoSi2-HGTS) surfaces which are exposed for catalyst placement by PVD or electroless deposition. CNTs have been grown selectively from those patterned areas. However, the yield and alignment of CNTs are not comparable with that achieved on planar substrates, possibly due to low density of catalyst particles. In order to achieve greater control over selectivity and density of catalyst deposition, another HGTS is designed and still under fabrication, where the vertical surface is electrically connected to facilitate selective electrochemical catalyst deposition. Furthermore, CNT growth from CoSi-HGTS is also investigated. CoSi is expected to be more catalytically active than CoSi2 as demonstrated by growth on planar substrates.

82

Theoretical study of the electronic structure of cubane-fullerene hetero-molecular crystals

Viktor Zólyomi¹ János Koltai² Jenő Kürti² Sándor Pekker¹

We present a first principles study of the electronic structure of cubane- C_{60} heteromolecular crystals, using density functional theory at the local density approximation level. The band structure is calculated along high symmetry lines and compared to that of the fcc C_{60} . We also present a study of the effect of possible potassium-doping as suggested by recent experiments. We find potassium doping to have a similar effect on the density of states in the cubane- C_{60} as in pure C_{60} , with a similarly high density of states at the Fermi level for the two materials. Charge transfer between the components of the studied materials is also calculated by Bader charge analysis. The possibility of a very small charge transfer between the cubane and

¹Department of Engineering, University of Cambridge, UK

²IMEC, Kapeldreef 75, B-3001, Belgium

¹Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Budapest

²Department of Biological Physics, Eötvös University, Budapest

Thursday, March 6

Poster session

the C_{60} in the undoped cubane- C_{60} hetero-molecular crystal is discussed.

Poster session Thursday, March 6

SINEUROP Nanotech GmbH



Private R&D Lab in Stuttgart

Founded by Siegmar Roth and his Team www.sineurop-nanotech.com

NANOTUBE PRODUCTION

single and multi
ARC DISCHARGE
LASER ABLATION
CHEMICAL VAP DEPOS

Development of Applications

Transparent Conducting Films Electromagnetic Shielding Heating Elements Composites

COOPERATIONS

Fraunhofer TEG Stuttgart Max Planck Inst f Festkörperforschung

Nanotech Alliance:

SINEUROP Nanotech GmbH Stuttgart Danubia NanoTech s.r.o. Bratislava Shanghai Yangtze Nanomaterials Co., Ltd. Nanomedical Sciences, Winston-Salem, NC

Quantum Interactions

8:30 – 9:00	L. Forró, CH Electron Spin Resonance of carbon-based nanostuctures
9:00 – 9:30	M. Mann, UK Device Electronics Based on Nanowires and Nanotubes
9:30 - 10:00	J. Morton, UK
	Switchable $ErSc_2N$ rotor within a C_{80} fullerene cage: an EPR and PL study
10:00 – 10:30	Coffee break
10:30 – 11:00	K. Ensslin, CH Graphene single electron transistors
11:00 – 11:30	C. Winkelmann, FR Optical Switching of Porphyrin-Coated Silicon Nanowire
11.00 10.00	Field Effect Transistors
11:30 – 12:00	B. Dora, DE Spin Gap and Luttinger Liquid Description of the NMR Re- laxation in Carbon Nanotubes
12:00 – 17:00	Mini Workshops
17:00 – 17:30	K. Holczer, US Single Electron Spin Microscope: the prospects of adding che-
17:30 – 18:00	$mical\ information\ to\ Atomic\ Force\ Microscope\ images.$
	W. Harneit, DE Detection of single electron spins in $N@C_{60}$ molecules
18:00 – 18:30	T. Pichler, DE IWEPNM 2008 - Conference Summary

20:00 Bauernbuffet - Farewell

Friday, March 7

Electron Spin Resonance of carbon-based nanostuctures

László Forró

Inst. of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne

The first step in creating devices where electron spin propagates the information is to find the suitable material where spin states have a long life-time. Carbon-based materials, with low spin-orbit coupling and low-dimensionality, such as single-wall carbon nanotubes (SWCNTs), endohedral fullerenes (e.g., $N@C_{60}$ or $X@C_{82}$, where X is a transition metal) encapsulated in SWNTs are ideal candidates. The progress in the ESR studies and measuring methods of these materials will be presented. Acknowledgment: This work is performed in collaboration with Luka Ciric, Arnaud Magrez, Andrzej Sienkiewicz, Mark Ruemmeli, Thomas Pichler, Hans Kuzmany, Jamie Warner and Andrew Briggs. It is supported by the European network IM-PRESS.

9:00

Device Electronics Based on Nanowires and Nanotubes

Maria Merlyene De Souza
¹ <u>Mark Mann</u>² Abbes Tahroui² William I Milne² Giuseppe Iannaccone³ Hans Kosina
⁴ Y Zhang²

¹Electronic and Electrical Engineering, University of Sheffield, UK

Electron devices based on quasi one dimensional channels are considered as the most promising candidates among emerging research devices to push the limits of integrated circuits beyond the limits of CMOS technology. Their main advantages include room temperature operation, suppression of short channel effects and promising perspectives for bottomup fabrication techniques.

Described will be integrated experimental and theoretical investigation of transport and noise in electronic devices based on single-walled carbon nanotubes CNTs and silicon nanowires. This will include a detailed description of the fabrication of top-gate and back-gate transistors, together with measurements and theoretical simulations of various electrical characteristics from 30 mK 450 K. Initial experimental measurements have indicated an FET on-off ratio of $10\hat{6}$. Simulation, atomic force microscopy and Raman spectroscopy have been employed to determine certain characteristics.

The doping effects of N2H4 and SbCl6 and the role of defects will also be discussed, together with the band structure measured for CNTs of varying chiralities. Finally, recent results of a new low-temperature CNT growth process will be presented which has been used to grow CNTs on CMOS devices already fabricated . Devices show little or no change in electrical characteristics after fabrication.

²Electrical Engineering Division, Cambridge, Cambridge

³IEEIIT-CNR, Pisa, Italy

⁴Institute for Microelectronics, TU Vienna, Austria

Switchable $ErSc_2N$ rotor within a C_{80} fullerene cage: an EPR and PL study

<u>John J. L. Morton</u>¹ Archana Tiwari¹ Geraldine Dantelle¹ Kyriakos Porfyrakis¹ Arzhang Ardavan² G. Andrew D. Briggs¹

¹Dept. of Materials, Oxford University, Parks Rd., Oxford, OX1 3PH, UK

Photoswitchable structural phenomena have been observed in range of organic and inorganic species and are essential processes in nature, with switching times as short as a picosecond. Natural photoisomerisation (such as bleaching of rod and cone retinal pigments in sight) has been exploited to engineer optical switches which can be used to store information and stimulate neurons. Fullerenes have been shown to provide remarkable nanovoids in which atoms, ions and molecules can exhibit nearly-free behaviour within a solid state environment. Examples include the quantisied rotational states in $C_2Sc_2@C_{84}$ and the exceptionally narrow electron paramagnetic resonance (EPR) lines of atomic nitrogen in $N@C_{60}$. It is common for such endohedral fullerenes to possess several stable structural isomers, though no evidence of photoisomerisation in such systems has thus far been reported.

Here we report the EPR signature of $\rm Er^{3+}$ within $\rm ErSc_2N@C_{80}$, making this the first endohedral ion known to be directly excitable both by EPR and optical techniques, and showing two primary configurations of the $\rm ErSc_2N$ unit within the fullerene cage. The relative populations of the two primary configurations can be manipulated optically: the excess of one configuration, obtained by thermal anealing, is converted into an excess of the other under illumination. The switching speed and reversibility of this photoisomerisation are yet to be determined; however, the long lifetime (over 12 hours at 20 K) of the switched orientation may find application in molecular memory elements.

10:30

Graphene single electron transistors

Christoph Stampfer 1 Johannes Güttinger 1 Francoise Molitor 1 Thomas ${\rm Ihn}^1$ Klaus ${\rm Ensslin}^1$

¹ETH Zurich, Switzerland

Graphene flakes are patterned into nanostructures using electron beam lithography and dry etching. A mesoscopic Hall bar is investigated by low-temperature magnetotransport experiments. The potential inside the Hall bar is tuned by graphene side gates. We demonstrate that the carrier density can be tuned over typical lateral distances of 90 nm. This way a tunable graphene single electron transistor is realized. Clear conductance resonances and Coulomb diamonds are resolved at a temperature of T=2 K. We present data for several graphene single electron transistors and discuss the tunability of the tunnel barriers as well as the overall electronic configuration of the device.

²Clarendon Laboratory, Oxford University, Parks Rd., Oxford, OX1 3PU, UK

Optical Switching of Porphyrin-Coated Silicon Nanowire Field Effect Transistors

C.B. Winkelmann¹

We study porphyrin derivative coated silicon nanowire field effect transistors, which display a large, stable and reproducible conductance increase upon illumination.[1] The efficiency and the kinetics of the optical switching are studied as a function of gate voltage, illumination wavelength and temperature. The decay kinetics from the high- to the low-conductance state is governed by charge recombination via tunneling, with a rate depending on the state of the SiNW-FET. The comparison to porphyrin sensitized Carbon Nanotube FETs allows to distinguish the environment- and molecule-dependent photoconversion process from the charge-to-current transducing effect of the semiconducting channel. (1) C.B. Winkelmann et al., Nano Lett. 7, 1454 (2007).

11:30

Spin Gap and Luttinger Liquid Description of the NMR Relaxation in Carbon Nanotubes

Ferenc Simon¹ Hans Kuzmany² Miklos Gulacsi³ Balazs Dora³

¹Budapest University of Technology and Economics, Institute of Physics and Condensed Matter Research Group, Hungarian Academy of Sciences, Post Office Box 91, H-1521 Budapest, Hungary

 2 Fakultat fuer Physik, Universitat Wien, Strudlhofgasse 4, A-1090 Wien, Austria 3 Max-Planck-Institut fuer Physik komplexer Systeme, Dresden

Recent NMR experiments by Singer et al. [1] showed a deviation from Fermi-liquid behavior in carbon nanotubes with an energy gap evident at low temperatures. Here, a comprehensive theory for the magnetic field and temperature dependent NMR ¹³C spin-lattice relaxation is given in the framework of the Tomonaga-Luttinger liquid. The low temperature properties are governed by a gapped relaxation due to a spin gap (30 K), which crosses over smoothly to the Luttinger liquid behavior with increasing temperature.

1 Singer et al., Phys. Rev. Lett. 95, 236403 (2005).

¹Institut Neel - CNRS/UJF Grenoble France

Friday, March 7

Quantum Interactions

Quantum Interactions

Friday, March 7

Single Electron Spin Microscope: the prospects of adding chemical information to Atomic Force Microscope images.

Karoly Holczer

UCLA, Department of Physics, Los Angeles, CA, USA

A successful combination of Magnetic Resonance with Scanning Probe Microscopy promises an atomic scale analytical tool. Single Electron Spin Microscope, i.e. a microscope with a single electron spin probe, is conceived to provide an atomic scale topographic image of a sample surface, while simultaneously identifying and investigating paramagnetic centers near the surface. Two features make SESM radically different from other Magnetic Resonance Force Microscope approaches: the use of a single-spin as a probe, and the possible room temperature operation. Over the past years the complex instrumentation with the required core performance has been assembled; the progress made in the realization will be reviewed from the perspective of the original concept.

17:30

Detection of single electron spins in N@C₆₀ molecules

Wolfgang Harneit

Freie Universität Berlin

For scalable solid-state or molecular spin-based quantum computers, the detection and coherent manipulation of single electron spins is mandatory. Due to its uniquely shielded configuration, the nitrogen atom encapsulated in an endohedral fullerene, N@C $_{60}$, provides a precisely locatable electron spin system with long coherence times. At the same time, the shielding makes access to the spin information exceedingly difficult.

We have investigated three methods to detect and manipulate single electron spins in $N@C_{60}$, optically detected magnetic resonance (ODMR), pulsed electrically detected magnetic resonance (pEDMR) and quantum transport in $N@C_{60}$ single molecule transistors (SMTs).

 $N@C_{60}$ has no allowed optical transitions in the visible, prohibiting direct access to its spin state via ODMR, but the spin state of N-V centers in diamond can be read out easily at room temperature. Small (~ 30 nm) diamond particles surrounded by $N@C_{60}$ fullerenes exhibit a spectroscopic splitting that could however not be uniquely assigned to $N@C_{60}$ molecules. We have observed similar spectra on diamond samples without $N@C_{60}$, and attribute the splitting to 13C atoms in the vicinity of the N-V center.

In pEDMR of (non-endohedral) C_{60} thin films, we observed coherent Rabi oscillations at room temperature, which we assign to $\tilde{}$ 10⁴ electron spins originating from defect-related states. Transferring the results to a smaller number of spins and to N@C₆₀ is experimentally difficult, but seems feasible in principle. Using this

approach has the advantage of combining spin detection and manipulation in a conventional setup.

In N@C $_{60}$ SMT devices, we observed a low-spin to high-spin transition in electron tunneling spectra at low temperatures. Theoretical calculations accounting for the antiferromagnetic exchange interaction between the neutral N spin and the spin of its charged C $_{60}$ cage reproduce this and other features. This allows us to identify the charge and spin states of the molecule, a first in SMT-probed molecular magnetism.

Austing, D. G., 17 Abrasonis, G., 92 Achiba, Y., 140 Avdeev, , 51 Adebimpe, D., 159 Avouris, P., 79 Agnello, S., 51 Ayala, P., **54**, 159, 171 Ajayan, P. M., 76, 138, 139 Akachi, T., 175, 179 Babaa, M., 99 Aksenov, V., 51 Bachmatiuk, A., 54 Bachtold, A., 47 Albrecht, M., 177 Alemipour, Z., 56 BAIBARAC, M. , 98Alessi, A., **51** Balestro, F., 176 Alexandre, S. S., 53 BALTOG, I., 98 Alig, A., 164 Bandow, S., 147 Alig, I., 98 Banki, P., 134 Alloul, H., 23 Bantignies, J., **55**, 99 ALMAIRAC, R., 52 BANTIGNIES, J. L., 52 Alvarez, L., 55 Bao, X., 111 ALVAREZ, L., 52 Baresova, V., 87 Alvermann, A., 68 Barjon, J., 83 Barros, E. B., 22 Alves, E. S., 131 Ando, T., 139 Basko, D. M., 69 Anikeeva, O. B., 95 Baxendale, M., 56 Anisimov, A. S., 171 Behrends, J. , 161Ansaldo, A., **52**, 155 Belli, M., 130 Araujo, P. T., **53**, 150 Bellouard, Y., 75 Ardavan, A., 154, 172, 175, 179, 188 Belova, E. E., 53Arnold, K., 79 Bennett, P., 81 Benyei, G., 134 Arnold, M. S., 79 Arstila, K., 67 Berndt, M. , $92\,$ Artyukhov, V. I., 53 Bianco, S., 137 Arutyunyan, N., 90, 128 Bilek, M. M. M., 92 Attacalite, C., 159 Bischof, R., 151 Blatt, S., 56, 174 Attaccalite, , 30 Attal-Tretout, B., 105 Blume, R., 177

Index

D 1 11 M 49 69	Cl N.D. 107
Bockrath, M., 42 , 62	Champness, N. R., 107
Boczkowski, J., 58	Chandra, B., 170
Bokor, M., 134	Charlier, J., 41
Bonnot, A., 105	Chassaing, D., 171
Borondics, F., 23, 141, 170	Cheng, Q., 61 , 66
Borowiak-Palen, E., 54, 57	Chernov, A., 113
Boscaino, R., 51	Chernov, A. I., 146
Bostwick, A., 162	Chernozatonskii, L. A., 53
Bouchiat, V., 176	Chevalier, X., 176
Brant, J. C., 131	Chiashi, S., 62
Bresson, L., 74, 128	Chiodarelli, N., 181
Breyer, C., 71	Chiu, H., 62
Briggs, A., 64	Chorro, M. C., 63
Briggs, G., 154	Chuvilin, A., 109
Briggs, G. A. D., 107, 172, 175, 179, 188	Ciric, L. D., 64
Brose, K., 173	Clavijo, C., 144
Bruckner, M., 23	Clemens, M. , 64
Brunner, J., 35	Cochon, J., 105
Bucher, C., 176	Corzilius, B., 65
Buechner, B., 159	Cott, D., 157, 181
BUISSON, J., 98	Cotte, M., 58
Bulusheva, L. G., 57 , 74, 148	Crochet, J., 64
Buryakov, T. I., 95	Csanyi, G., 60
Bushueva, E. G., 148	Cudzilo, S., 82
Busiakiewicz, A., 82	, ,
Bussy, C., 58	da Silva, A. J. R., 34
Büchner, B., 161	Dabrowski, P., 82
Byrne, H. J., 61, 66	Dalton, A., 66
, , , ,	Dantelle, G., 154, 172, 188
Calame, M., 35	Das, A., 18
Calandra, M. , 160	Davis, R. C., 78
Cambedouzou, J. , 58 , 63	Debnath, S., 61
Cantoro, M., 133, 177	Debnath, S., 66
Carlsson, J. M., 59	Dehm, S., 132
Casiraghi, C., 60	Dettlaff-Weglikowska, U., 67, 153
Castellarin-Cudia, C., 133	Dianov, E., 113
Cau, M., 105	Dietzel, A., 75
Caudal, N., 18, 73	Dinse, K., 65
Cech, J., 88	Doorn, S. K., 53, 150
Cepek, C., 133	Dora, B., 23, 189
Cervantes-Sodi, F., 60, 81	Dorfmüller, J., 18
Chacham, H., 53	Dorval, N., 105
Chacon, C., 128	Dossot, M., 165
Chamberlain, T. W., 107	Doucet, J., 58
, · · · , ± • ·	

Dresselhaus, M. S., 22, 86	Fuchsbauer, A., 142
Drucker, J., 81	Fujiki, S., 140
DSouza, F., 94	Fukushima, T., 43
Ducastelle, F., 83	Futaba, D. N. , 78
Ducati, C., 81, 177	, , ,
Duncan, A., 64	Gadermaier, C., 72
Dunin-Borkowski, R., 81	Galland, C., 73
Dunsch, L., 72	Gauckler, J., 85
Durrer, L., 47, 166	Gava, P., 73
Duffer, L., 47, 100	Ge, L., 175
Eberhardt, W. E., 30	Gebert, A., 161
Edwards, D. M., 68	Gelardi, F. M., 51
Einarsson, E., 68 , 91	Germing, T., 159
Elias, D. C., 131	Gendt, S. D., 157
Emtsev, K. V., 97, 157, 162	George, C., 155
Endo, M., 22, 150	Georgi, C., 16, 153
Engel, M., 98	Gevko, P., 74
Enouz, S., 55, 128	Gingl, Z., 76, 80, 139
Ensslin, K., 75, 166, 188	Giorcelli, M., 137
Ermolov, V., 180	Goetz, G., 74
Exnar, I., 88	Goffredi, A., 130
	Gokus, T., 16, 60
Falko, V., 35	Goldhaber-Gordon, D., 167
Farhat, H., 86	Goldoni, A., 133
Fazzio, A., 34	Goncalves, G., 142
Fehske, H., 68	González, T. , 35
Ferrari, A. C., 60, 69 , 169	Govindaraj, A., 18
Ferreira, M., 70	Graetzel, M., 88
Ferreira, M. S., 152	Graf, D., 75
Ferrer-Anglada, N., 70	Graupner, R., 97, 157
Fiawoo, M., 105	Grebenyukov, V., 90
Filho, A. G. S., 22	Green, A. A., 72, 153
Fink, J., 30	Gregan, E., 61
Finnie, P., 17	Grigoras, K., 180
Fischer, J., 112	Grodzka, E., 94
Forró, L., 23, 64, 130, 135, 172, 187	Grove-Rasmussen, K., 83
Fort, Y., 165	Grüneis, A., 30 , 77
Fostiropoulos, K., 71, 161	Gulacsi, M., 189
Fouquet, M., 170	Gusinski, A. V., 95
Franck, B., 143	Guthy, C., 112
Frank, O., 72	Güttinger, J., 75 , 188
Franssila, S., 180	
Freitag, M., 43	Haddon, R. C., 23
Fromherz, T., 142	Haevecker, M., 177
, -·, <u>-</u>	,,,,,

Halonen, N., 80, 139 Hung, P., 62 Haluška, M., **75**, 82, 145 Iannaccone, G., 187 Hambach, R., 91 Ihn, T., 75, 188 Han, S., 76 Iijima, S., 147 Hanashima, T., 62 Hanke, F., 59 Ilani, S., 31 Harima, H., 89 Imamoğlu, A., 73 Harneit, W., 141, 161, 192 Inderbitzin, K., 166 Hart, A. J., 76 Ionescu, R., 76, 80 Ionica, I., 176 Hartschuh, A., 16, 53, 60, 153 Ischenko, A. V., 95 Harutyunyan, H., 16, 60 Ishii, H., 140 Haspál, H., 139 Itkis, M. E., 23 Haspel, H., 76, 80, 93 Hata, K., 53, 65, 78, 120 Ito, Y., 175, 179 Hayamizu, Y., 78 Iwasiewicz-Wabnig, A., 63 Hedderman, T. G., 66 Jaffrennou, P., 83 Heinz, T. F., 15, 170 Jakab, E., 141 Helbling, T., 47 Hennrich, F., 16, 78, 84, 132 Jalsovszky, I., 134 Jester, S., 84, 89 Herges, R., 158 Hermite, M. M. 1., 58 Jiang, H., 171 Jin, Z., 89 Hersam, M. C., 16, 72, 79, 124, 153 Johansson, A., 156 Hertel, T., 64, 79 Hesser, G., 142 Jonkman, H. T., 34 Heszler, P., 76, 80, 139 Jørgensen, H. I., 83 Heyns, M., 157 Jorio, A., 53, 85, 150 Hierold, C., 47, 85, 166 Joung, S., 147 Hildebrandt, P., 173 JOURDAIN, V., 52 Hirado, Y., 140 Jozsa, C., **34** Hirsch, A., 108, 137, 149 Jungen, A., 85 Hirtschulz, M., 80, 131 Kaippinen, E. I., 146 Hofmann, S., 81, 133, 177 Kaiser, A. B., 86, 164 Holczer, K., 192 Kaiser, U., 109 Högele, A., 73 Homma, Y., 62 Kakehi, H., 89 Kalbac, M., 86 Hone, J., 170 Kalbacova, M., 87 Horn, K., 162 Kalenczuk, R. J., 54 Hsu, C., 167 Huard, B., 30, 167 Kamar, K., 170 Huber, R., 35 Kamaras, K., 23, 93, 141, 149 Huczko, A., 82 Kanahori, K., 62 Kappes, M., 79 Hulman, M., 82, 151 Kappes, M. M., 78, 84, 89 Humbert, B., 165 Hundhausen, M., 157 Kasama, T., 81

V-t II 110 140	Vl. D. C. 119
Kataura, H., 119 , 140	Kryukov, P. G., 113
Katkov, V. L. , 87	Kuemmeth, F., 31
Kauppinen, E., 54	Kukovecz, A, 139
Kauppinen, E. I., 171, 180	Kukovecz, A., 76, 80, 93 , 151
Kavan, L., 72, 86, 88	Kulmala, T., 180
Kern, K., 18	Kuntscher, C., 170
Khlobystov, A. N., 107	Kuntscher, C. A., 93
Kim, Y. A., 22	Kurenya, A. G., 57
Kinloch, I., 57	Kürti, J., 90, 96 , 181
Kiowski, O., 84, 89	Kusar, P., 72
Kiricsi, I., 80, 93	Kutner, W., 94
KISODA, K., 89	Kuzhir, P. P., 95
Kleshch, V., 90	Kuzmany, H., 23, 54, 107, 150, 151, 189
Klupp, G., 170	Kuznetsov, V. L., 95
Klusek, Z., 82	Kuznetsov, V. V., 148
Klymenko, Y., 162	Kyzyma, , 51
Kmoch, S., 87	
Knob-Gericke, A., 177	Laake, L. v. , 75
Knoll, P., 150	Lagerwall, J. P. F., 160
Knorr, A., 80, 131	Lagoute, J., 128
Köck, A., 151	Lanone, S., 58
Kodama, T., 140	Lanzani, G., 79
Kolitsch, A., 92	Lanzara, A., 29
Koltai, J., 90 , 96, 181	Lastra, J. M. G., 152
Kong, J., 86	Laszlo, I., 96
Konov, V., 113	Lau, C. N. (., 97
Kónya, Z. , 76, 80, 93, 139	Lauffer, P. , 97
Korbely, B., 130	Launois, P., 58, 63
Kordás, K., 76, 80, 138, 139	Lauret, J., 128
Korecz, L., 172	Lauret, J. S., 83
Korobov, , 51	Lavayen, V., 144
Koshino, M., 91	Lazzeri, M., 18, 73, 160, 173
Kosina, H., 187	Lebedkin, S., 78, 84, 89
Kouwenhoven, L., 74	Leccia, E., 58
Kovats, E., 134	Lee, W., 100
Kowalczyk, P., 82	Lefebvre, J., 17
Kozlowski, W., 82	Lefrant, S., 147
Kramberger, C., 91 , 159, 166	LEFRANT, S., 98
Krasheninnikov, A., 67	Lellinger, D., 98 , 164
Krause, M., 92	Lenormand, F., 55
Krenn, J., 151	Leon, V., 99
Kriza, G., 134	Leonhardt, A., 161
Kromka, A., 87	LEPARC, R., 52
Krupke, R., 56, 132, 174	Leturcq, R., 166
•	

Ley, L., 97, 157	Mceuen, P. L., 31
Li, C., 167	
	McRae, E., 165
Li, Y., 89	Mehring, M., 141
Liang, C., 100	Meissner, D., 142
Lidorikis, E., 60	Mele, E. J., 129
Lin, F., 167	Melle-Franco, M., 107
Lin, H., 128	Mende, J., 141
Lindelof, P. E., 83	MENENDEZ, J., 22
Lips, K., 161	Mertig, M., 155
Lobach, A., 113, 128	Meshot, E. R., 76
Lobach, A. S., 146	Meunier, V., 22
Loiseau, A., 74, 83, 105 , 128	MEVELLEC, J., 98
Louie, S. G., 29	Meyer, C., 166
Lüer, L., 79	Michalikova, L., 87
Luzzi, D. E., 129	Michel, K. H., 134
	Mihailovic, D., 72, 106 , 168
Machón, M., 158	Milde, F., 80, 131
Maciel, I. O., 53, 85	Milne, W. I., 187
Maex, K., 157	Minett, A., 112
Mafra, D. L., 131	Mingesz, R., 76, 80
Magrez, A., 130 , 135	Mionic, M., 135
Maguer, A., 128	Miyahara, T., 140
Makarova, T. L., 130	Miyata, Y., 119
Mäklin, J., 76, 80, 138, 139	Miyauchi, Y., 136
Maksimenko, S. A., 95	Mizuno, K., 78
Malard, L. M., 131	Moeller, W., 92
Malić, E., 80, 131	Mohr, M., 137
Malysheva, L., 149	Moilanen, H., 80, 139
Mamane, V., 165	Molitor, F., 75, 188
Maniwa, Y., 119, 140	Molodtsov, S., 30, 77
Mann, M., 187	Monthioux, M., 63
Margez, A., 64	Morton, J. J. L., 172, 188
Marini, A., 159	Moseenkov, S. I., 95
Marquardt, C. W., 132	Moshammer, K., 84
Maruyama, S., 68, 91, 125 , 136	Müller, M., 137
Matsumoto, K., 89	Munnik, F., 92
Matt, G. J., 142	Murakami, T., 89
Mattevi, C., 133	
Matus, P., 134	Muramatsu, H., 22
	Musso, S. , 137
Maultzsch, J., 131, 137, 170	Mustonen, T., 76, 80, 138 , 139
Mauri, F., 73	Nafradi B 22 64 179
Mauri, F., 18 , 160, 173	Nafradi, B., 23, 64, 172
Mazzani, M., 130	Nagatsu, K., 62
McChesney, J., 162	Naito, R., 89

N.1	D 15 405
Nakamura, E., 91	Pavese, M., 137
Nakanishi, T., 139 , 147	Pekker, A., 23, 141, 149
Nakatake, M., 140	Pekker, S., 134, 141, 181
Nakayama, Y., 44 , 140	Perebeinos, V., 79
Nam, C., 112	Perez-Puigdemont, J., 70
Nasibulin, A. G., 146, 171, 180	Pesce, P. B., 53
Naydenov, B. , 141	Pesce, P. B. C., 150
Negreira, A. R., 157	Peterlik, H., 107, 150
Nemeth, K., 141	Pfeiffer, R., 107, 150
Neto, A. H. C., 131	Pichler, T., 30, 54, 77, 91, 159, 161
Neugebauer, H., 142	Pierzchala, K., 64
Nicolas, R., 143	Pieta, P., 94
Nikolaev, P., 150	Pimenta, M. A., 53, 85, 131
Nilsson, J., 131	Pinault, M., 58
Noe, L. N. , 63	Piscanec, S., 60, 69
Novoselov, K. S., 60	Pivrikas, A., 142
Novotny, L., 16, 153	Plank, W., 151
Nozar, P., 174	Plentz, F., 131
, , , ,	Ploscaru, M., 168
Obergfell, D., 82, 109, 145	Polanski, K., 82
Obraztsov, A., 90	Pontiroli, D., 130
Obraztsova, E., 90, 113, 128	Popinciuc, M., 34
Obraztsova, E. A., 147	Porfyrakis, K., 154, 172, 175, 179, 188
Obraztsova, E. D. , 146 , 147	Postma, H., 62
ODwyer, C., 144	Pötschke, P., 98, 164
Oesterreich, A., 177	Pouillon, Y., 152
Ogura, K., 68	POWELEIT, C., 22
Ohta, T., 162	Power, S. R., 152
Okada, S. , 147	Pozharov, A., 90
Okawa, J. , 68	Pressl, K., 150
Okazaki, T., 147	Pugno, N., 137
Okimoto, H., 175, 179	0 , ,
Okotrub, A. V., 74	Qian, H., 16, 53, 60, 153
Okotrub, A. V., 57, 148	Quintavalle, D., 23, 172
Okubo, S., 147	, , ,
Olejniczak, W., 82	Rafailov, P. M. , 153
Olevik, D., 165	Rahman, R., 154
Onipko, A., 149 , 162	Ralph, D. C., 31
Osadchy, A. V., 147	Ranjan, N., 155
Otani, M., 147	Rao, A. M., 85
Oze, M., 93	RAO, A. M., 22
	Rao, C. N., 18
Parodi, M. T. , 155	RAO, P. B. , 55
Pasquarello, A., 178	RAO, R., 22

Reich, S., 80, 131	Sariciftci, N. S., 142
Reinning, L., 91	Sato, K., 78
Rellinghaus, B., 159, 161	SAUVAJOL, J. L., 52
Repain, V., 128	Scalia, G., 82, 160
Resasco, D. E., 23	Scardaci, V., 169
Rezek, B., 87	Schönenberger, C., 35
Ricci, D., 52, 155	Schaefer, S. , 161
Ricco, M., 130	Schaeffel, F., 159
Richter, M., 131	Schaeffer, B., 93
Rinkiö, M., 156	Scheffler, M., 59
Rinzler, A. G., 23	Schenderlein, M., 173
Robertson, J., 81, 119 , 133, 177, 181	Schloegl, R., 177
Roch, N., 176	Schneider, C. M., 166
Rocha, A. R., 34	Schnoerch, P., 177
Rodrigues, O. E. D., 22	Schultz, L., 159, 161
Rogala, M., 82	Schäffel, F. , 161
Röhrl, J., 157	Schünemann, C., 161
Rols, S., 63	SCOTT, L. T. , 52
Roman, C., 47	Sedelnikova, O. V., 57
Romanenko, A. I., 95	Serge, F., 143
Roppert, K., 151	Seyller, T., 97, 157, 162
ROSE, J., 52	Sharma, R., 81, 177
Rosenkranz, N., 158	Shenderova, O. A., 95
Rossi, M., 34	Shevtsov, A., 162
Rosta, , 51	Shinohara, H., 175, 179
Rotenberg, E., 162	Shiozawa, H., 140, 163
Roth, S., 52, 67, 70, 82, 100, 109, 145,	Sienkiewicz, A., 64
153, 155, 160, 164	Simon, F., 23 , 93, 150, 172, 189
Rousset, S., 128	Sitter, H., 142
Royal, G., 176	Skakalova, V., 67, 86, 164
Rozhin, A. G., 169	Skipa, T., 164
Rubio, A., 30, 152, 159	Smajda, R., 93
Rümmeli, M. H., 159 , 161	Snegir, , 51
Ruhavets, O. V., 95	Soldatov, A. V., 165
Russo, R. M., 129	Song, H., 57
Ryves, L., 92	Sood, A. K., 18
10,700, 21, 02	Souza, M. M. D., 187
Saito, R., 78	Spitsina, N., 128
Saito, T., 147	Spudat, C., 166
Saitoh, T., 140	Staddon, L., 107
Saitta, A., 18, 73	Stadler, P., 142
Saitta, A. M., 160	Stafström, S., 149, 162
Samsonidze, G., 131	Stampfer, C., 75, 85, 166 , 188
Saremi, S., 161	Stander, N., 167
1 1	

Steele, G., 74 Steiner, M., 53	Tsukagoshi, K., 31 Tureci, H., 73
Steplewska, A., 54	III 1 M 140
Stobinski, L., 167	Ullah, M., 142
Strano, M. S., 125	Uplaznik, M., 168
Strle, J. , 168	Vähäkangas, J. , 80 , 139
Stürzl, N., 84	Vajtai, R., 76, 138
Suenaga, K., 91	Vajtaj, R., 139
SUENAGA, K. , 120	Vandecasteele, N., 173
Sulpizio, J., 167	Vengust, D., 72, 168
Sun, Z., 169	Venukadasula, G. M., 94
Sundqvist, B., 63	Verberck, B., 134
Tagliaferro, A., 137	Vereecken, P., 157, 181
Tahroui, A., 187	Verploegen, E., 76
Taliani, C., 174	Vigolo, B., 165
Tan, Y., 23	Vijayaraghavan, A., 56, 132, 174
Tanner, D. B., 23	Vincent, B., 143
Täschner, C., 161	Vogelgesang, R., 18
Tausenev, A., 113	Vos, W., 74
Telg, H., 170	Vretenar, V., 174
Terrones, H., 85	Vyalikh, D., 30, 77
Terrones, M., 22, 85, 121	Warm E 160
Teschner, D., 177	Wang, F., 169
Tham, D., 112	Warner, J. 4, 64 Warner, J. H. 175, 170
Thirunavukkuarasu, K., 93, 170	Warner, J. H., 175 , 179 Watt, A. A. R., 172, 175, 179
Thomsen, C., 80, 137, 153, 158, 170, 173	Wees, B. J. v., 34
Tian, Y., 171	Wernsdorfer, W., 176
Tiwari, A., 154, 172 , 188	Whelan, C., 181
Todd, K., 167	White, I. H., 169
Tombros, N., 34	Winkelmann, C., 176 , 189
Tompa, K., 134	Winkler, K., 94
Toppari, J., 156	Wirth, C. T., 81, 133, 177
Törmä, P., 156	Wirtz, L., 159
Torres, C. M. S., 144	Wolfgang, W., 143
Toth, G., 80, 138	Wu, S., 35
Toth, S., 23, 172	Wu, Y., 170
Tóth, G., 139	Wunderlich, D., 137, 149
Tress, W., 71	Wzietek, P., 23
Tretout, B. A., 83	W: D 40
Tripisciano, C., 57 Tropin, 51	Xiang, R., 68
Tsai, C., 100	Yakobson, B. I., 48
Tschirner, N., 173	Yamada, T., 78
100000000000000000000000000000000000000	I aiii aa a

Index

Yaminsky, I. V., 147 Yanagi, K., 119 Yazyev, O. V., **178** Yumura, M., 78 Yushina, I., 74

Zafeiratos, S. , 177
Zaka, M. H. , 175, 179
Zavodchikova, M. , 156
Zavodchikova, M. Y. , 146, 180
Zerbetto, F. , 107
Zettl, A. K. , 105
Zhang, C. , 181
Zhang, Y. , 187
Zhang, Z. , 68
Zitti, E. D. , 155
Zouni, A. , 173
Zólyomi, V. , 90 , 96, 181