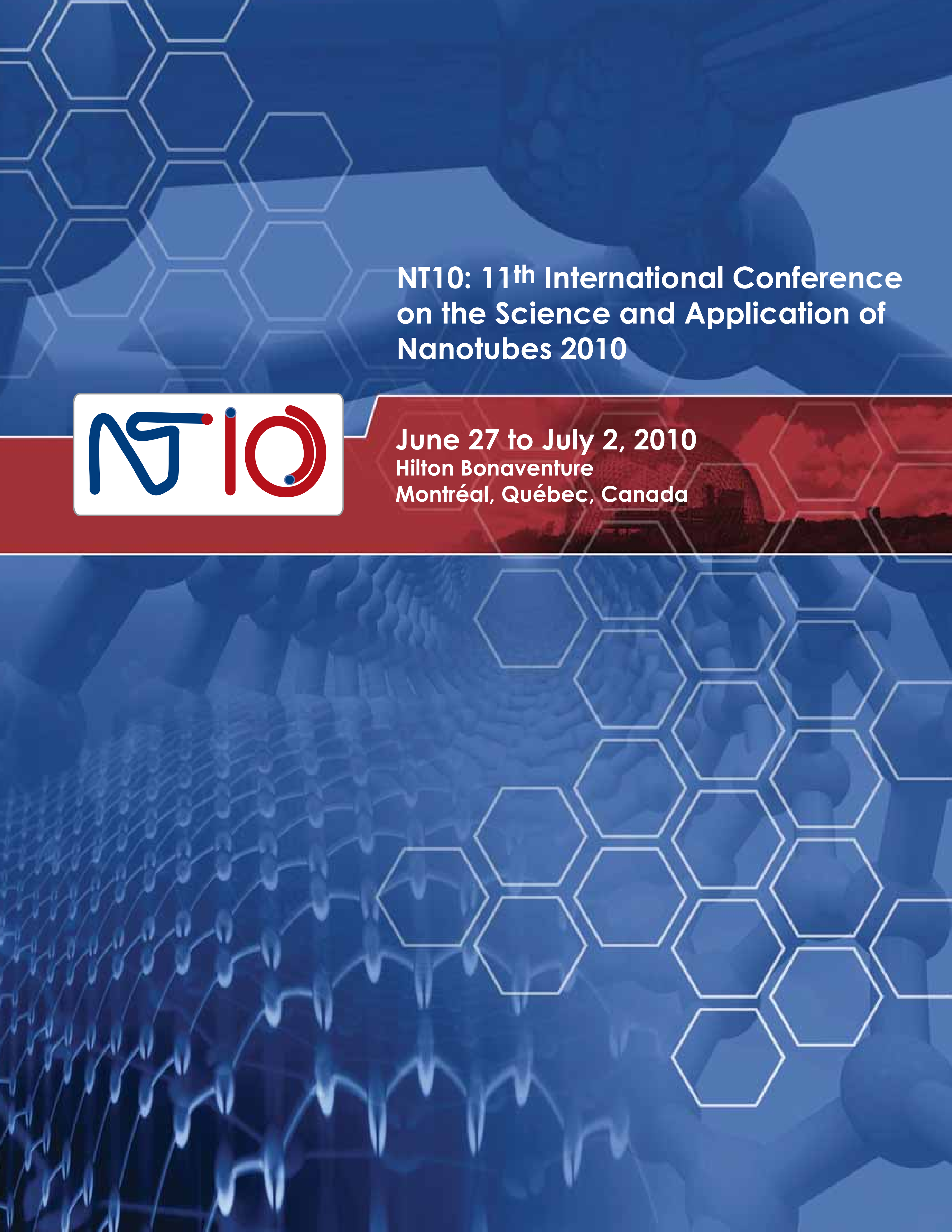

# NT10: 11th International Conference on the Science and Application of Nanotubes 2010

June 27 to July 2, 2010
Hilton Bonaventure
Montréal, Québec, Canada

| | Sunday, June 27th | Monday, June 28th | Tuesday, June 29th | Wednesday, June 30th | Thursday, July 1st | Friday, July 2nd |
|---|---|---|---|---|---|---|
| 8:00 | Registration | | Opening Remarks | | | |
| 8:30 | Satellite Workshops: CCTN10, MSIN10, CNBMT10, GSS10 | Satellite Workshops: CCTN10, GSS10 | K1 - R. Baughman | K2 - A. Geim | K4 - Y. Homma | K5 - L. Dai |
| 9:10 | | | CT1 - C. Gibon<br>CT2 - C. Zhi<br>CT3 - K. Kobashi | CT13 - D. Kondo<br>CT14 - T. Heinz<br>CT15 - X. Ling | CT21 - B. Liu<br>CT22 - E. Einarsson<br>CT23 - V. Jourdain | CT33 - S. Fogden<br>CT34 - H. Liu<br>CT35 - A. Adronov |
| 9:27 | | | | | | |
| 9:44 | | | | | | |
| 10:01 | Coffee Break | Coffee Break | Poster Session 1 | Poster Session 3 | Poster Session 4 | Poster Session 6 |
| 10:20 | Satellite Workshops: CCTN10, MSIN10, CNBMT10, GSS10 | Satellite Workshops: CCTN10, GSS10 | | | | |
| 11:30 | | | IT1 - J.-C. Chartier | IT4 - J. Delgado | IT5 - A. Imamoglu | IT8 - S. Torti |
| 11:55 | Lunch | Lunch | CT4 - A. Loiseau<br>CT5 - B. Neves | CT16 - L. Ortolani<br>CT17 - C. Spataru | CT24 - A. Johansson<br>CT25 - E. Gaufres | CT36 - T. Martinez<br>CT37 - E. Flahaut |
| 12:29 | | | | | | |
| 13:00 | Satellite Workshops: CCTN10, MSIN10, CNBMT10, GSS10 | Satellite Workshops: CCTN10, GSS10<br>Tutorial A | Lunch | Lunch | Lunch | Lunch |
| 14:00 | | Tutorial B | IT2 - M. Strano | K3 - P. McEuen | IT6 - A. Harutyunyan | IT9 - A. Bianco |
| 14:25 | | | CT6 - P. Collins<br>CT7 - G. Buchs<br>CT8 - B. Goldsmith<br>CT9 - W. Wenseleers | | CT26 - C. Huynh<br>CT27 - C. Kingston<br>CT28 - K. Koziol<br>CT29 - J. Zhang | CT38 - K. Ihara<br>CT40 – T.Saito |
| 14:49 | Coffee Break | Coffee Break | | CT18 - D. Cobden<br>CT19 – A. Bushmaker<br>CT20 - J. Lehman | | |
| 14:59 | | | | | | |
| 15:00 | Satellite Workshops: CCTN10, MSIN10, CNBMT10, GSS10 | Satellite Workshops: CCTN10, GSS10<br>Tutorial C | | | | IT10 - M. Zheng |
| 15:16 | | | Poster Session 2 | Free Time | Poster Session 5 | Summary |
| 15:33 | | | | | | |
| 16:00 | | | | | | Closing Remarks |
| 16.20 | | Tutorial D | | | | |
| 16:30 | | | | | | |
| 17:00 | | | IT3 - R. Saito | | IT7 - S. Purcell | |
| 17:25 | | | CT10 - S. Doorn<br>CT11 - A. San Miguel | | CT30 - T. Yamada<br>CT31 - M. Itkis<br>CT32 - C. Zhou | |
| 17:30 | | | Tribute | Excursion and Banquet | | |
| 17:59 | | | | | | |
| 18:30 | | Welcome Reception | | | | |
| 20:30 | | | | | | |
| 23:00 | | | | | | |

**Legend:**

| | |
|---|---|
| CT | Contributed Talk |
| IT | Invited Talk |
| K | Keynote Speaker |

# Table of Contents

# Committees and Organization

## NT10 Organizing Committee

**Richard Martel** (Department of Chemistry, Université de Montréal)

**Paul Finnie** (Institute for Microstructural Sciences, National Research Council Canada)

**Jacques Lefebvre** (Institute for Microstructural Sciences, National Research Council Canada)

**Benoit Simard** (Steacie Institute for Molecular Sciences, National Research Council Canada)

## NT10 Advisory Board

Prof. A. Windle (Cambridge University, United Kingdom)
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Dr. M. Yudasaka (AIST, Japan)

## NT10 Conference Secretariat - JPdL

1555 Peel, Suite 500
Montréal, Québec H3A 3L8
Canada
nt10-montreal@jpdl.com
www.jpdl.com

# Welcome from the NT10 Organizing Committee

The NT10 Organizing Committee would like to welcome you to NT10: the Eleventh International Conference on the Science and Application of Nanotubes 2010, held at the Hilton Bonaventure in downtown Montréal, Québec, Canada.

NT10 is the 11th in the NT conference series started with NT99 in Michigan, USA and now running annually and rotating between the Americas, Asia, and Europe. The NT conference is the largest international forum for researchers to discuss the latest developments in nanotube science and technology. From its modest beginning as a reasonably small workshop the NT conferences have grown steadily in participation and in complexity. Today, NT10 has received more than 700 abstract submissions.

As in past NT conferences, NT10 puts a special emphasis on the poster sessions with a total of over 500 contributed posters divided into approximately a dozen themes. In addition to the contributed poster sessions, five (5) keynote and ten (10) invited speakers were selected by the results of a vote by the NT Advisory Committee. From the contributed abstracts, 40 contributed talks were selected on the basis of their excellence, novelty and field of research. The number of contributed talks was increased considerably this year in an effort to better reflect the large number of contributed abstracts, but still only about 6% of contributed abstracts could be presented orally.

NT10 has no parallel sessions per se, but in addition to the general program there are four satellite workshops, held on the first two days of the NT10 conference, each with their own organizing committees, selection processes, and web presence:

- **CCTN10**: the 6th International Symposium on Computational Challenges and Tools for Nanotubes
- **MSIN10**: the 4th International Workshop on Metrology, Standardization and Industrial Quality of Nanotubes
- **CNBMT10:** the 3rd Carbon Nanotube Biology, Medicine and Toxicology Satellite Symposium
- **GSS10**: the 1st Graphene Satellite Symposium (new)

In addition to the satellite workshops, there is a tutorial session intended to bring graduate students up to date with the latest in nanotube research. All these workshops are free to NT10 participants.

It takes tremendous resources to put on an event of this size and complexity. The NT10 Organizing Committee would like to express its gratitude to NanoQuébec, Université de Montréal and the National Research Council Canada, each of which provided support for the organization of NT10 on a completely not-for-profit basis. We would like to thank the organizers of the satellite workshops and the advisory committee for their efforts assembling such great NT10 programs and the volunteers who helped the NT10 organization. Finally, we thank our many sponsors and exhibitors who provided financial support to the success of NT10 and JPdL for logistic support.

Ultimately, it is you, the participants, who make NT such a lively and interesting meeting. We are grateful to you for coming from all parts of the world to share your work and attend the meeting. Over 600 of you have come because of your enthusiasm for this remarkable field of research, which is now vibrant and full of potential.

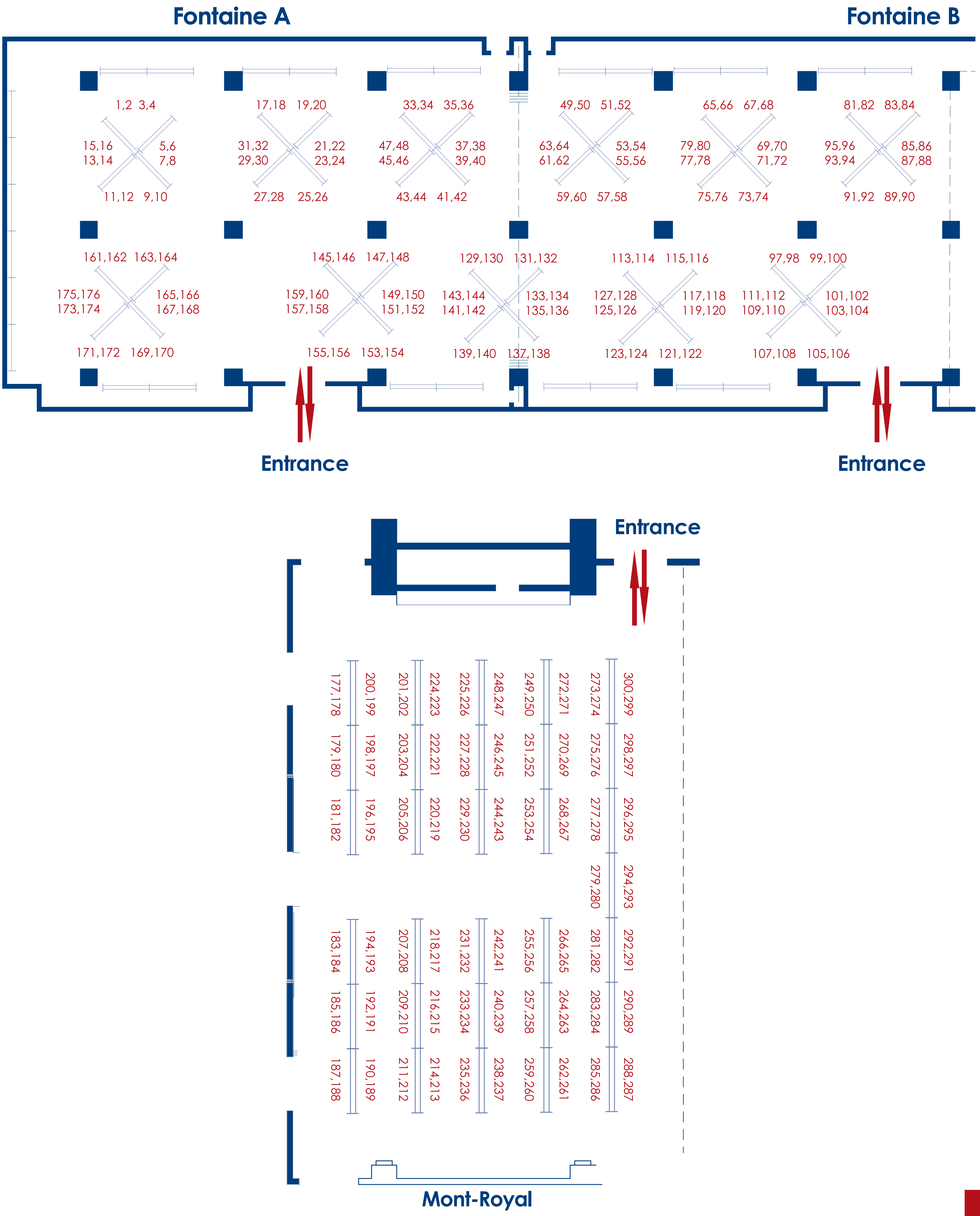
The city of Montréal is situated at the confluence of two great rivers, and is of tremendous importance in the history of North America. Today it is a diverse, modern city and we welcome you and hope you will enjoy exploring its neighbourhoods and/or attending to its 31st edition of the Festival International de Jazz de Montréal. We hope NT10 will be a very successful conference for you. May you learn and contribute to the exciting field of nanotube science and application.

Sincerely,

**The NT10 Organizing Committee**

- **Richard Martel,**
  *Department of Chemistry,*
  *Université de Montréal*
- **Paul Finnie,**
  *Institute for Microstructural Sciences,*
  *National Research Council Canada*
- **Jacques Lefebvre,**
  *Institute for Microstructural Sciences,*
  *National Research Council Canada*
- **Benoit Simard,**
  *Steacie Institute for Molecular Sciences,*
  *National Research Council Canada*

# Poster Session Floor Plan



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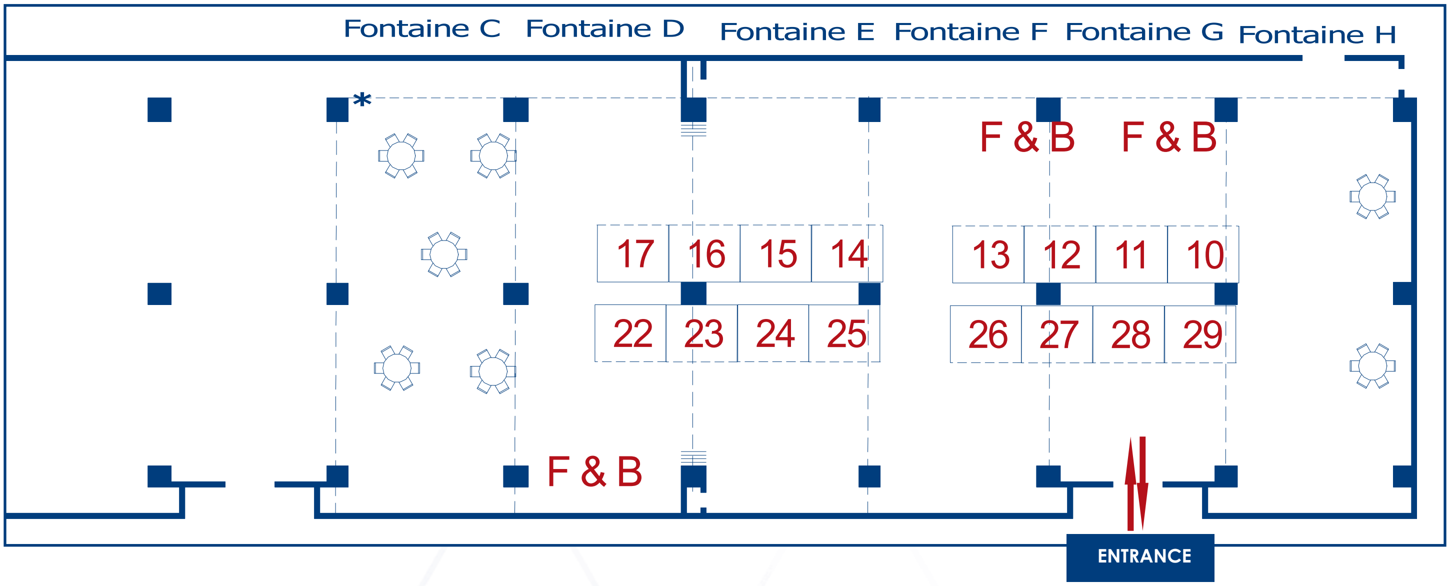


## List of Exhibitors

**Aixtron** ............ 15
AIXTRON is a leading provider of deposition equipment to the semiconductor industry. The Company's technology solutions are used by a diverse range of customers worldwide to build advanced components for electronic and opto-electronic applications based on compound, silicon, or organic semiconductor materials, as well as Carbon Nanotubes(CNT) and other nanomaterials. Such components are used in fiber optic communication systems, wireless and mobile telephony applications, optical and electronic storage devices, computing, signalling and lighting, as well as a range of other leading-edge technologies.

**Betatek** ............ 10
Distributor of laboratory equipment manufactured throughout the world. Our core market consists of Pharmaceutical Marketing companies operating in Canada.

**Delong America and Soquelec Ltd** ............ 14
Soquelec Ltd and Delong are supplying the research and industrial community with state of the art equipment for Materials and Life Sciences. The Delong LVEM5 is the next generation of electron microscope, built on a revolutionary technology platform that combines advanced imaging with unparalleled benchtop convenience. The LVEM5 Benchtop Electron Microscope is the smallest multi-mode desktop electron microscope and the only Benchtop TEM on the market today.

**Delta Photonics** ............ 12
Delta Photonics is a leading Canadian photonics distributor for scientific research, aerospace & defense, industrial, OEM and biomedical applications. We deliver the best solutions for lasers, light sources, spectroscopy systems, imaging cameras, micro-Raman, AFM/NSOM, radiometric and photometric instruments, high quality optical components and precision opto-mechanical hardware.

**Nanofactory Instruments AB** ............ 23
Nanofactory Instruments is the world leader in providing specialized SPM systems (STM, AFM, NanoIndenter) designed to work in TEM. these unique SPM-TEM instruments provide unprecedented opportunity to combine 3 dimensional nanomanipulation, STM-AFM imaging and in-situ electrical and mechanical probing with high resolution TEM imaging.

**NanoIntegris** ............ 28
NanoIntegris, a spin out form Professor Mark Hersam's research group from Northwesterm University, produces 99% enriched semiconducting and 99% enriched metallic SWNTs. Recently, NanoIntegris launched single and double layer graphene nanoplatelets. To date, NanoIntegris has over 100 academic and industrial customers around the world, and NanoIntegris customers have published in Nature Nanotechnology, ACS Nano, Nano letters, Applied Physics Letters, and JACS.

**NanoQuebec** ........................................ 25
NanoQuebec's Major Central Facilities Network (MCFN) regroup aeven research infrastructures for the fabrication and analysis of nanomaterials and nanodevices. Accessible to all academic and industrial users, the MCFN fosters research in nanotechnology and provides solutions for the industry.

**NRC/CNRC** ........................................ 26
The National Research Council (NRC) is the Government of Canada's premier organization for research and development and is a centrepiece of Canada's innovation system. NRC provides an integrated approach for the synthesis, characterization, metrology and the chemical integration of carbon nanotubes, through to the fabrication and prototyping of real-world applications. NRC also assists its clients with product validation and regulatory approval.

**Olympus Canada** ........................................ 29
Olympus industrial microscopes and metrology systems play a leading role in precision, R&D engineering &manufacturing applications in fields such as aerospace, automotive industry, electronics, materials science metallurgy, medical devices & semi conductors.

**Omicron** ........................................ 27
Omicron NanoTechnology is the world's leading supplier of analytical instrumentation in nanotechnology R&D. We create innovative and tailored solutions and uniquely combine thin-film techniques with sophisticated Multi-Technique analytics into integrated UHV-systems. Some Omicron Highlights: The largest UHV Scanning Probe Microscope range with benchmark performance; MBE, PVD, ALD, PLD and More to Creating Tomorrow's Materials Today!; 3 nm UHV SEM & 5 nm SAM à "NanoSAM Lab"; Ultimate electrical probing on sub-10nm structures à "UHV Nanoprobe"; Atomic Resolution nc-AFM at 5 K à "MULTIPROBE LT".

**Photon etc** ........................................ 13
Photon etc. is a Canadian company developing and manufacturing spectral analysis instruments From UV to NIR our patented optical fillering technology allow us to offer state of the art hyper spectral imaging laser lunable fillers, and widely lunable filters, and widely lunable lasers. Founded In 2002 by Sebastien Blala-Ouellelle while working at the California Institute of Technology, Photon ect is both en RD company and a specialized manufacturer of advanced instruments.

**Plasmionique** ........................................ 16
Plasmionique Inc is a Canadian company at forefront of technological development for tools and processes used in Thin, Film Processing, Surface Engineering and advanced Material Synthesis (including CNT) applications, using Plasma, Laser and Vacuum-based technologies.

**Renishaw Inc** ........................................ 11
Renishaw Raman spectrometers are configurable to include multiple excitation sources from the UV through NIR with automated laser switching and alignment, quick-launch fiber-optic probes, AFM/NSOM/Raman, SEM-Raman, hot/cold cells, macrosampling, global Raman imaging, near excitation analysis, 2D/3D mapping and depth-profiling. Renishaw Raman spectrometers provide chemical/molecular information confocally and can be configured for sub-micron spatial resolution with options for auto-alignment, internal calibration & performance validation.

**Systems for Research** ........................................ 24
Systems for Research Corp is the exclusive Canadian Sales and service Representative for many premier manufacturers of surface characterization and materials analysis. Techniques include Electron Microscopy, XPS, Scanning Probe Microscopy. Please visit www.sfr.ca for more information.

## Exhibit Hall Schedule

### Tuesday June 29

| | |
|---|---|
| 07:00 - 08:30 | Poster setup |
| 09:30 | Opening of Exhibition |
| 10:00 - 10:30 | Coffee Break |
| 10:00 - 11:30 | Poster Session 1 |
| 12:30 - 14:00 | Lunch |
| 15:30 – 16:00 | Refreshment Break |
| 15:30 - 17:00 | Poster Session 2 |
| 17:00: | Exhibition closes |

### Wednesday June 30

| | |
|---|---|
| 09:30 - 10:30 | Exhibition opens |
| 10:00 - 10:30 | Coffee Break |
| 10:00 - 11:30 | Poster Session 3 |
| 12:30 - 14:00 | Lunch |
| 12:30 – 14:00 | Poster take-down |
| 17:00 | Exhibition closes |

**Meals During the Exhibition**
Delegates are invited to enjoy all refreshment breaks and lunches in the exhibit hall.

**Thursday July 1**

| | |
|---|---|
| 07:00 - 08:30 | Poster setup |
| 09:30 | Exhibition opens |
| 10:00 - 10:30 | Coffee Break |
| 10:00 - 11:30 | Poster Session 4 |
| 12:30 - 14:00 | Lunch |
| 15:30 - 16:00 | Refreshment Break |
| 15:30 - 17:00 | Poster Session 5 |
| 17:00 | Exhibition ends |

**Friday July 2**

| | |
|---|---|
| 10:00 - 11:30 | Poster Session 6 |
| 10:00 - 10:30 | Coffee Break |
| 12:30 - 14:00 | Lunch |
| 12:30 – 14:00 | Poster take-down |

# Useful Information, Delegate Services

## Useful Information

### Welcome Reception

Monday, June 29, 18:00-20:00, Hilton Bonaventure Hotel
All conference delegates are invited to the Welcome Reception, taking place at the Hilton Bonaventure.

### Excursion and Banquet:
### Dinner Cruise on the Saint Lawrence River

Board this spectacular cruise ship at nightfall and cast off for a few hours of pure escape on the mighty Saint Lawrence River. Departing from King Edward pier in the Old Port, you can take in the lights of Montreal from the unmatched viewpoint of the fully glassed-in dining rooms. Add to this the luscious dinner concocted by our chef and a festive atmosphere aboard, and you have all the ingredients for a perfect evening.

Inclusions: Cruise with 5-course meal, cocktail, wine service during dinner.

*Timeline:*

| | |
|---|---|
| 18:00 | Boarding and Cocktail (King Edward Pier) |
| 19:00 | Departure and Conference Banquet |
| 23:00 | Back to King Edward pier |

### *Transportation to and from King Edward Pier (Old Montreal):*

| | |
|---|---|
| By Foot: | 2.4 km from Hilton Bonaventure (30-minute walk) |
| Metro: (subway) | Place Bonaventure to Place d'Armes (2 stations) + 7-minute walk from Place d'Armes metro to King Edward pier |
| Taxi: | Taxis available in front of the Hilton Bonaventure (departure) and on De la Commune Street (return) |

### Exchange and Banking Facilities

Banks and bank machines (automatic tellers) can be found throughout the city. Regular banking hours are 10:00 to 17:00, Monday to Friday, with extended hours including weekends at some locations. Currency exchange offices are plentiful in the downtown core. Main branches of Canadian banks are equipped to exchange foreign currency as well. Most banks have automatic teller machines (ATM), which can be accessed 24 hours a day, using bank or credit cards on major international banking networks such as Cirrus, Plus and Interac. Credit cards and debit cards are used more commonly than cash except in the case of small amounts.

### Official Conference Hotel

**Hilton Bonaventure**
900, de la Gauchetière Ouest
Montréal, Québec H5A 1E4
Phone: 1-514-878-2332
Metro Station (subway): Bonaventure (orange line)
www.hilton.com

### Language

French is the official language of the Province of Québec. English is mother tongue of a significant fraction of the population in and around Montréal, and downtown Montréal is essentially very bilingual (French and English). English is spoken and understood in almost all downtown locations serving visitors, including airports, hotels, tourist attractions, shops and restaurants.

# Delegate Services

## Registration – Schedule

| | |
|---|---|
| Saturday, June 26 | 14:00 – 18:00 |
| Sunday, June 27 | 07:30 – 18:30 |
| Monday, June 28 | 07:30 – 19:00 |
| Tuesday, June 29 | 07:00 – 18:30 |
| Wednesday, June 30 | 07:30 – 18:00 |
| Thursday, July 1 | 07:00 – 18:30 |
| Friday, July 2 | 07:30 – 16:30 |

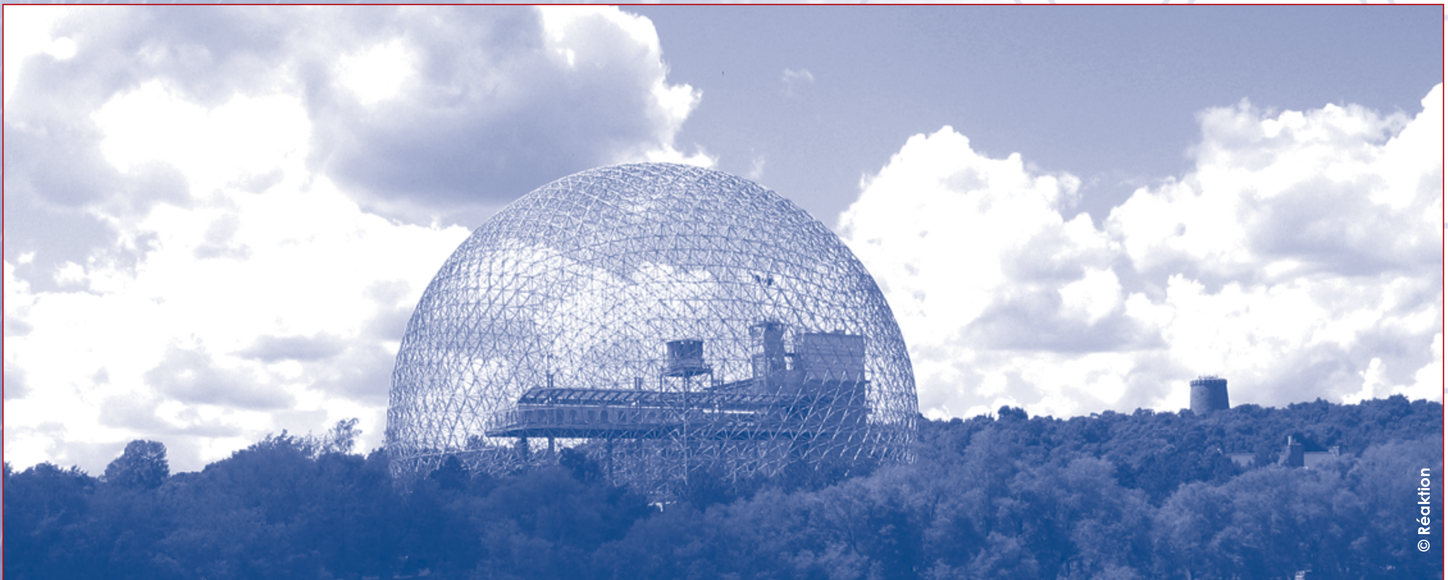
## Secretariat – Schedule

| | |
|---|---|
| Saturday, June 26 | Closed |
| Sunday, June 27 | 07:00 – 18:00 |
| Monday, June 28 | 07:30 – 19:00 |
| Tuesday, June 29 | 07:00 – 18:00 |
| Wednesday, June 30 | 07:30 – 18:00 |
| Thursday, July 1 | 07:00 – 18:00 |
| Friday, July 2 | 07:30 – 16:00 |

## Transportation

The City of Montréal offers an extensive public transit system, including Metro (subway), trains and buses. The orange and green metro lines serve the city centre. The Hilton Bonaventure hotel is situated by Bonaventure metro station (orange line). Single fare is $2.75 CAD or $13.25 by pack of 6 tickets. Tourist cards are available in all metro stations for a daily unlimited use at $7 or $14 for a three-day use. Opening hours are 05:30 to 01:00 (the blue line closes at 00:15). To see schedules and fare options, visit the STM – Société de transport de Montréal website: www.stm.info/index.htm.

Taxis are plentiful and can be hailed from the street or at the airport, train and bus stations. Fares begin at $3.30 CAD.



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# Satellite Workshops and Tutorial Program

## 6th International Symposium on Computational Challenges and Tools for Nanotubes 2010 (CCTN10)

**Organizers:**
**Alain Rochefort**, *Department of Engineering Physics, Polytechnique Montréal*
**Hishashi Nakamura**, *Research Organization for Information Science & Technology (RIST)*
**Stephan Roche**, *Commission de l'Énergie Atomique (CEA)*

## ROOM: OUTREMONT

## Sunday, June 27

### 8:30-8:40

**Welcoming Remarks of the CCTN10 Committee**
**Alain Rochefort**

### ■ *Radiation and Irradiation*

### 8:40-9:20 Invited Speaker

**Biomimetic Color Detection Using Chromophore-Nanotube Hybrid Devices**
**François Léonard**, *Sandia National Laboratory, USA*

Phototransduction plays a central role in key natural processes such as vision and photosynthesis. For these processes, natural evolution has found exquisite solutions that optimize efficiency, compactness, and self-healing. While researchers have long tried to supplant nature's successes using solid-state approaches, our ability to convert optical radiation to electrical signals with nanoscale precision still remains in its infancy. An alternative to solid-state approaches is one that more closely mimics natural processes by integrating chemical or biological materials with solid-state materials. To this end, we present a nanoscale color detector based on a single-walled carbon nanotube functionalized with azobenzene chromophores, where the chromophores serve as photoabsorbers and the nanotube as the electronic read-out. By synthesizing chromophores with specific absorption windows in the visible spectrum and anchoring them to the nanotube surface, we demonstrate the controlled detection of visible light of low intensity in narrow ranges of wavelengths. Our measurements suggest that upon photoabsorption, the chromophores isomerize from the ground state trans configuration to the excited state cis configuration, accompanied by a large change in dipole moment, changing the electrostatic environment of the nanotube. We will also present our all-electron ab initio calculations that are used to study the chromophore-nanotube hybrids and show that the chromophores bind strongly to the nanotubes without disturbing the electronic structure of either species. Calculated values of the dipole moments support the notion of dipole changes as the optical detection mechanism.

### 9:20-9:40 Contributed Talk

**Surface electromagnetic phenomena in pristine and atomically doped carbon nanotubes**
**Igor Bondarev**, *North Carolina Central University, USA*

This talk reviews recent theoretical effort towards understanding the near-field optoelectronic properties of pristine and atomically doped carbon nanotubes. The research is motivated by the progress in the growth techniques of centimeter-long small-diameter single-walled nanotubes[1], measurements of the excitonic photoluminescence[2], experiments on the encapsulation of single atoms into single-walled nanotubes[3], and finally by the need for the development of materials that may host quantum coherent states with long coherence lifetimes[4]. A variety of electromagnetic phenomena, such as atomic spontaneous decay dynamics[5], atom-nanotube van der Waals coupling[6] and inter-tube Casimir attraction[7],[8], light absorption[9] and entanglement of extrinsic atoms (ions)[10] doped into carbon nanotubes, exciton-plasmon interactions[11] and optical response of surface exciton-plasmons in individual nanotubes[12], as well as their potential applications in nanophotonics and nanoplasmonics, will be discussed. Supported by NSF (HRD-0833184), NASA (NNX09AV07A), and ARO (57969-PH-H). [1]L.Zheng et al., Nature Materials 3,673(2004). [2]M.S.Dresselhaus et al., Annu. Rev. Phys. Chem. 58,719(2007).[3]G.-H.Jeong et al, Phys. Rev. B 68,075410(2003). [4]T.Brandes, Phys. Rep. 408, 315 (2005). [5]I.V.Bondarev and Ph.Lambin, Phys. Rev. B 70,035407(2004). [6]I.V.Bondarev and Ph.Lambin, Phys. Rev. B 72,035451(2005). [7]A.Popescu, L.M.Woods, and I.V.Bondarev, Phys. Rev. B 77, 115443 (2008). [8]A.Popescu, L.M.Woods, and I.V.Bondarev, Phys. Rev. Lett., submitted. [9] I.V.Bondarev and B.Vlahovic, Phys. Rev. B 74,073401(2006). [10] I.V.Bondarev and B.Vlahovic, Phys. Rev. B 75,033402(2007).[11] I.V.Bondarev, L.M.Woods, and K.Tatur, Phys. Rev. B 80,085407(2009). [12]I.V.Bondarev, K.Tatur, and L.M.Woods, Optics Commun. 282,661(2009).

### 9:40-10:00 Contributed Talk

**Modeling irradiation effects on graphene using quantum molecular dynamics**
**Eduardo Cruz-Silva**, *Oak Ridge National Lab, USA* | **Zachary M. Barnett**, *Oak Ridge National Lab, USA* | **Andres Botello-Mendez**, *Oak Ridge National Lab, USA* | **Humberto Terrones**, *Oak Ridge National Lab, USA* | **Mauricio Terrones**, *Oak Ridge National Lab, USA* | **Bobby G. Sumpter**, *Oak Ridge National Lab, USA* | **Vincent Meunier**, *Oak Ridge National Lab, USA*

Graphene is a promising material for nanoelectronic devices, but the fulfilling of its promise relies on the control of its thickness and edge shape, which affect their electronic properties. Electron irradiation has been proposed as a method to exfoliate graphene, which combined with Joule heating edge reconstruction provides control over both thickness and edge shape. Using a combination of molecular dynamics and density functional theory, we present a study of electron irradiation effects in the dynamics of graphene bilayers. We also present the effects of these irradiation induced defects in the quantum transport properties of graphene. Our results show that irradiation induced defects are responsible for modifying the edge dynamics and provide a new method for tailoring graphene atomic structure at the nanoscale.

### Coffee Break

### ■ *Charge Transport*

### 10:30-11:10 Invited Speaker

**Conductance of functionalized nanowires, nanotubes and graphene**
**Xavier Blase**, *Institut Néel, CNRS and UJF, France* | **Marivi Fernandez-Serra**, *Dept. of Physics and Astronomy Stony Brook University, NY* | **François Triozon**, *CEA/LETI, Grenoble, France.* | **Alejandro Lopez-Bezanilla**, *CEA/INAC, France* | **Blanca Biel**, *CEA/INAC, France* | **Stephan Roche**, *CEA/INAC, France*

We review in this presentation recent theoretical work aiming at understanding the impact of doping and functionalization on the transport properties of silicon nanowires [1], nanotubes [2] and graphene [3,4]. Based on ab initio calculations (DFT-Landauer formalism) we show that while in general the random modification of the conducting channel destroys quickly the conductance of 1D systems, strategies can be found to limitate, or exploit, the negative impact of random doping and functionalization. We show further that ab initio calculations can address the problem of the conductance of micrometer long tubes with hundreds of grafted molecules, bridging thus the gap between ab initio and mesoscopic physics. [1] Fernandez-Serra and Blase, Phys. Rev. Lett. 100, 046802 (2008). [2] Lopez-Bezanilla et al., NanoLetters 9, 940944 (2009). [3] Biel et al., Phys. Rev. Lett. 102, 096803 (2009). [4] Lherbier et al., Phys. Rev. Lett. 101, 036808 (2008).

## 11:10-11:30 Contributed Talk

### Electron transport of meso-scale carbon nanotube-based materials at the finite temperature

**Syogo Tejima**, *Research Organization For Information Science & Technology, Japan* | **Satoshi Nakamura**, *Research Organization For Information Science & Technology, Japan* | **Hisashi Nakamura**, *Research Organization For Information Science & Technology, Japan* | **David Tomanek**, *Michigan State University*

We have investigated electron transport of carbon nanotube at the finite temperature through the large scale simulation using high-end supercomputer. For our research, we have developed an advanced tight-binding molecular dynamical method based on a non-equilibrium Green's function at the finite temperature for simulating the electrical conduction through electrodes. Avoiding heavy loads in computing, our O(N) approach of algorithm enables us to simulate the meso-scale electrical quantum transport phenomena with several ten thousands of carbon atoms. It results that the current flux at each atomic point of a single-walled nanotube strongly depends on the condition of electrodes to which the carbon nanotube is connected at both ends. As the quantum effect on current flux, it shows that the relation of current-voltage is distinct from that of the classical transport defined by Ohm's law. The difference gradually disappears with increasing temperature because the quantum effect is weakened. In addition to a single walled nanotube, we will discus the electron transport properties of a double wall and twisted bundle carbon nanotubes.

## 11:30-11:50 Contributed Talk

### Percolation in size distributed carbon nanotubes mats

**Louis-Philippe Simoneau**, *Engineering Physics Department and Regroupement québécois sur les matériaux de pointe (RQMP), École Polytechnique de Montréal, Canada* | **Alain Rochefort**, *Engineering Physics Department and Regroupement québécois sur les matériaux de pointe (RQMP), École Polytechnique de Montréal, Canada*

Carbon nanotubes mats (CNTMat) with various degrees of structural organization have promising electric properties that compare with those of actual transparent electrodes used in electroluminescent and photovoltaic devices. The optimization of such complex materials and the description of the underlying physics can be efficiently addressed by computational means. For example, the modeling of charge transport in such complex systems improves our understanding of the influence of the network structure on the quality of the electrode, and contributes to selectively optimized the electrode properties. The charge transport models already developed for CNTMat typically consider a single parameter to describe the tube-tube junctions [1]. However, it has been recently shown that the propagation of charge carriers is limited by contact resistance which is far from being unique in CNTMat where nanotubes have various physical properties [2]. We have developed Monte Carlo algorithms simulating the charge transport in bidimensional networks of carbon nanotubes that incorporate a realistic distribution and description of tube-tube junctions. The algorithms generate random networks, check for percolation paths and evaluate the total conductance of the CNTMat on the basis of individual contacts conductances, which in turn depend on the local network properties. We will present different results in which the importance of the nanotube distribution on the resulting electrical performances can be described in terms of length, diameter, orientation and chirality of the nanotube distribution within the percolative network. [1] J. Hicks et al., Phy. Rev. E, 79, (2009). [2] P. N. Nirmalraj et al. Nano Lett., 9, (2009).

## Lunch / Poster Session

## ■ *A Touch of Spin and Field*

## 13:40-14:00 Contributed Talk

### Emergence of local magnetic moments in doped graphene-related materials

**Mauro Ferreira**, *Trinity College Dublin, Ireland* | **Pedro Venezuela**, *Universidade Federal Fluminense, Brazil* | **Antonio Costa**, *Universidade Federal Fluminense, Brazil* | **Roberto Muniz**, *Universidade Federal Fluminense, Brazil* | **Stephen Power**, *Trinity College Dublin, Ireland* | **David Edwards**, *Imperial College, UK*

Motivated by recent studies reporting the formation of localized magnetic moments in doped graphene, we investigate the energetic cost for spin polarizing isolated impurities embedded in this material. When a well-known criterion for the formation of local magnetic moments in metals is applied to graphene we are able to predict the existence of magnetic moments in cases that are in clear contrast to previously reported Density Functional Theory (DFT) results. When generalized to periodically repeated impurities, a geometry so commonly used in most DFT-calculations, this criterion shows that the energy balance involved in such calculations contains unavoidable contributions from the long-ranged pairwise magnetic interactions between all impurities. This proves the fundamental inadequacy of the DFT-assumption of independent unit cells in the case of magnetically doped low-dimensional graphene-based materials. We show that this can be circumvented if more than one impurity per unit cell is considered, in which case the DFT results agree perfectly well with the criterion-based predictions for the onset of localized magnetic moments in graphene. Furthermore, the existence of such a criterion determining whether or not a magnetic moment is likely to arise within graphene will be instrumental for predicting the ideal materials for future carbon-based spintronic applications. [1] [1] Phys. Rev. B 80, 241413(R) (2009)

## 14:00-14:20 Contributed Talk

### Magnetotransport of carbon nanotubes devices: intrinsic vs. contact phenomena

**Georgy Fedorov**, *Russian Research Centre 'Kurchatov Institute', Russia* | **Alexander Tselev**, *Georgetown University, Washington, USA* | **Yanfei Yang**, *Georgetown University, Washington, USA* | **Jianyun Zhou**, *Georgetown University, Washington, USA* | **Makarand Paranjape**, *Georgetown University, Washington, USA* | **Paola Barbara**, *Georgetown University, Washington, USA* | **Dmitry Smirnov** | **David Jimenez** | **Sylvain Latyl** | **Stephan Roche**

Soon after discovery of carbon nanotubes (CNT), Ajiki and Ando [1] predicted that an axial magnetic field would tune the bandstructure of a CNT between a metal and a semiconductor. This effect is due to the modulation of the Aharonov-Bohm phase of the electronic wavefunctions and peculiar topology of the graphene's Fermi surface. Such ability to tune the bandstructure of a nanotube provides new opportunities to probe intrinsic properties of CNTs as well as properties of CNT-based nanodevices. Here we study effect of an axial magnetic field on transport properties of CNT-based gated devices with different geometry, electrode material and CNT type: metallic, quasi-metallic or semiconducting [2, 3]. We demonstrate that modification of the band structure has a strong effect on their transport characteristics. We show that a CNT device magnetoresistance can be calculated within a relatively simple phenomenological model based on Landauer-Buttiker formalism and an approximate expression describing the shape of the band profile of the device. This approach allows for restoring of the shape of the band profile. Finally we show that magnetotransport of quasi-metallic CNTs is very sensitive to the CNT chirality. That allows for identification of the chirality of the quasi-metallic CNTs in our devices. REFERENCES: [1] Ajiki, H. & Ando, T. J. Phys. Soc. Jpn. 62, 1255-1266 (1993) [2] Fedorov, G., Tselv, A., Jimenez, Latil, S., D., Kalugin, N., Barbara, P., Smirnov, D., Roche, S., Nano Letters, 7(4), 960-964, (2007) [3] Fedorov, G., Smirnov, D., Jimenez, D., Barbara P., Roche S., Appl. Phys. Lett. (2010)

### 14:20-14:40 Contributed Talk

**Spin polarization enhancement in disordered carbon-based systems**

**Alexandre Rocha**, *Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Brazil* | **Thiago B. Martins**, *Physics Institute, University of São Paulo, Brazil* | **James Ameida**, *Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Brazil* | **Adalberto Fazzio**, *Physics Institute, University of São Paulo, Brazil* | **Antônio José Roque da Silva,** *Physics Institute, University of São Paulo, Brazil; Laboratório Nacional de Luz Síncrotron, Brazil*

The possibility of using the spin of the electron instead of its charge can lead to a new family of devices. In the so called field of spintronics, the spin of the electron is the ultimate logic bit. In the quest to achieve this goal carbon nanotubes present themselves as possible candidates. In particular, nitrogen-rich carbon nanotubes – the so called CNx nanotubes – could be used as possible binding sites for magnetic impurities that could, in turn, result in spin polarized transport. In this work we show, by means of ab initio electronic transpor calculations, how these nitrogen-rich carbon nanotubes can be used as spintronics devices by incorporating transition metal ions. The resulting structure resembles that of Heme-B molecules which are the active sites in Hemoglobin and thus present in nature. The ions used in the present study, such as iron, cobalt and manganese, present a localized magnetic moment that leads to spin-dependent scattering. Using a combination of density functional theory and non-equilibrium Green's functions, we demonstrate that, in the presence of a large number of magnetic scattering centers the degree of spin polarization of the electronic conductance of initially unpolarized electrons entering the device can reach 100 %. We also show that these devices also present a very large giant-magnetoresistance-type effect when a small mangetic field is applied and the mangetic moments of the impurities is aligned. All these effects are explained in terms of the Anderson localization regime for a long and disordered one-dimensional system.

### 14:40-15:00 Contributed Talk

**Dynamic Alignment of Single-Walled Carbon Nanotubes in Pulsed Magnetic Fields**

**Nicolas Ubrig**, *Laboratoire Nationale Des Champs Magnétiques Intenses, France* | **Junichiro Kono**, *Department of electrical and computer engineering, Rice University* | **Matteo Pasquali,** *Department of chemical and biomolecular engineering, Rice University* | **Jeffrey Fagan**, *NIST, USA* | **Oliver Portugall**, *Laboratoire Nationale Des Champs Magnétiques Intenses, France*

The dynamic alignment allows the investigation of 2 fundamental physical properties of carbon nanotubes, i.e. the magnetic susceptibility through the total amount of aligned tubes in a liquid suspension and the dynamic behaviour of this tubes treated as rodlike particles. Semiconducting tubes are diamagnetic both along and perpendicular to their long axis but the magnitude of the perpendicular susceptibility is higher. Metallic tubes are paramagnetic along their long axis and diamagnetic perpendicular to it. This constrains SWNT to align parallel to a magnetic field. The brownian motion is the competing force against the external field and cause isotropic alignment in its absence. We investigate the alignment with linear dichroism, an accurate method due to the optical selection rules of carbon nanotubes which only absorbs light with an electric field vector parallel to the tube long axis. We compare the experimental data to a theoretical model based on rotational diffusion describing the dynamic parameters of the solution. The important parameters (e.g. length distributions, viscosities, etc...) of the sample are characterised with the help of AFM and rheological measurements. We thus can conclude the limits of validity of the model. From the maximum in linear dichroism we can calculate the anisotropy in the magnetic susceptibility. This results will be compared to earlier theoretical models and calculations[1,2]. Experiments on different chirality and samples lead to conclusions on diameter and length dependences of the magnetic anisotropy. [2] J.P.Lu, PRL 74, 1123 (1995) [3] H.Ajiki and T.Ando, J.Phys.Soc.Jpn. 64, 4382 (1995)

### Coffee Break

## ■ *Phonons and Vibrations - CCTN*

### 15:30-16:10 Invited Speaker

**Phonon populations and energy dissipation in carbon nanotube transistors: Experimental and computational challenges**

**Mathias Steiner**, *IBM Research Division, T. J. Watson, Research Center, USA*

Due to their favorable optical and electronic properties, single wall carbon nanotubes are promising for application in nano-photonics and optoelectronics. Optical spectroscopy and electrical transport measurements on the single nanotube level are among the challenges that have to be tackled experimentally. In addition, it has become more and more obvious that an increasing effort has to be put into data analysis and computational modeling in order to quantify and interpret the experimental results obtained. In this talk, I will show how the combination of electrical transport measurements and optical micro-spectroscopy can be used to probe phonon populations in a device made of a single carbon nanotube. The combination of experiment, data analysis and computational modeling reveals a comprehensive picture of electrical transport, phonon populations and dissipation pathways in a functioning carbon nanotube transistor [1]. [1] M. Steiner, M. Freitag, V. Perebeinos, J. C. Tsang, J. P. Small, M. Kinoshita, D. Yuan, J. Liu and Ph. Avouris, Nature Nanotechnology 4, 320-324 (2009)

### 16:10-16:30 Contributed Talk

**DC Excitation and Cooling of the Carbon Nanotubes Vibrations**

**Leonid Gorelik**, *Chalmers University Of Technology, Sweden* | **Fabio Santandrea** | **Robert Shekhter** | **Mats Jonson**

We have theoretically investigated electromechanical properties of freely suspended carbon nanotubes when a dc-current is injected into the tubes using a scanning tunneling microscope. We demonstrate that a shuttle-like electromechanical instability can occur if the bias voltage exceeds a dissipation-dependent threshold value. An instability results in large amplitude vibrations of the carbon nanotube flexural mode, which modify the current-voltage characteristics of the system. Then we show that at a certain bias voltage below the Coulomb blockade threshold the quantum interference effects controlling inelastic electronic tunneling result in an effective cooling of the nanotube vibrations. Our analysis, which is performed in the framework of the rate equations formalism, shows that such cooling is possible down to a ground state level where the average occupation number of the lowest flexural vibration mode of the nanotube is ~ 0.2

### 16:30-19:00 Poster Session

**The Initial Stages of SWCNT CVD Synthesis on SiO2 Nanoparticles: A QM/MD Investigation**

**Alister Page**, *Fukui Institute for Fundamental Chemistry, Kyoto University, Japan* | **Stephan Irle**, *Institute for Advanced Research and Department of Chemistry, Nagoya University, Japan* | **Keiji Morokuma**, *Fukui Institute for Fundamental Chemistry, Kyoto University, Japan; Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, USA*

The ability of non-metal catalysts, notably SiO2, to assist the nucleation and growth of SWCNTs via CVD has recently been established [1]. Speculations that the traditional VLS mechanism is possibly responsible for SWCNT nucleation on silica nanoparticles have also been made recently [2]. However, the exact mechanism by which SiO2 assists the nucleation and growth of SWCNTs remains unknown. In this work, we address this issue by simulating CH4 CVD on a SiO2 nanoparticle at 1200 K using QM/MD simulations. In contrast to CVD using traditional Fe-group catalysts, CVD on SiO2 induced a complex chemical process. Most notably, CO was produced as the primary chemical product via the carbothermal reduction of SiO2, a fact that is consistent with recent experimental observations [2]. Ultimately, the insertion of carbon into/removal of oxygen from the SiO2 nanoparticle resulted in the local formation of amorphous SiC. However, this carbothermal reduction was limited to the outer regions of the catalyst, with the core of the particle remaining predominantly composed of Si and O. On this basis, we suggest that a traditional VLS model of SiO2-catalyzed SWCNT nucleation may by inadequate. The formation of a SWCNT “nucleus” on the SiO2 surface was ultimately observed following further annealing at 1200 K. Interestingly, components of this mechanism are reminiscent of those found during Fe-catalyzed SWCNT nucleation [3]. [1] Y. Homma et al., Nano Res., 2009, 2, 793. [2] A. Bachmatiuk et al., ACS Nano, 2009, 3, 4098. [3] Y. Ohta, et al., ACS Nano 2009, 3, 3413.

### First-principles based kinetic modeling of effect of hydrogen on growth of carbon nanotubes

**Andrey Knizhnik**, *Kintech Lab Ltd, Moscow, Russia* |**Irina Lebedeva**, *Kintech Lab Ltd, Moscow, Russia* | **Alexey Gavrikov**, *Kintech Lab Ltd, Moscow, Russia* | **Alexey Baranov**, *Kintech Lab Ltd, Moscow, Russia* | **Maxim Belov**, *Kintech Lab Ltd, Moscow, Russia* | **Boris Potapkin**, *Kintech Lab Ltd, Moscow, Russia* | **Steven Aceto**, *GE Global Research Center, Niskayuna, New York, USA* | **Pierre-Andre Bui**, *GE Global Research Center, Niskayuna, New York, USA* | **Chris Eastman**, *GE Global Research Center, Niskayuna, New York, USA* | **Ulrike Grossner**, *GE Global Research Center, Niskayuna, New York, USA* | **David Smith**, *GE Global Research Center, Niskayuna, New York, USA* | **Tim Sommerer**, *GE Global Research Center, Niskayuna, New York, USA*

The influence of hydrogen on the separate stages of carbon nanotube growth is investigated for thermal chemical vapor deposition. According to our kinetic calculations, during the delivery of carbon precursors by the gas flow, the precursors can be hydrogenated, thus leading to modification of the carbon supply rate onto the catalyst particle. A simple kinetic model of growth of CNTs based on the first-principles calculations of kinetic parameters for dissociation of hydrocarbons on the catalyst surface is suggested to study the hydrogen-modified adsorption/desorption kinetics of precursors on the Ni (111) and Ni (113) surfaces. Using the proposed model, conditions at which the growth of CNTs is possible are analyzed. Hydrogen is shown to decrease the coverage of hydrocarbons and thus prevent deactivation of the catalyst. Density functional theory calculations reveal that hydrogen adatoms effectively bind to edges of graphitic structures on the Ni (111) surface. This leads to a significant decrease of the rate of carbon attachment to the growing graphitic structures. The results obtained are shown to be in good agreement with the experimental data.

### Computer simulation studies of Carbon Nanotube – catalyst particle interfaces

**Hakim Amara**, *Laboratoire d’Etude des MIcrostructures, Onera-Cnrs, France* | **Anders Börjesson**, *School of Engineering, University of Borås, Sweden and - Department of Physics, Gothenburg University,Sweden* | **Christophe Bichara**, *CINaM, CNRS, France* | **Kim Bolton**, *School of Engineering,University of Borås, Sweden and Department of Physics, Gothenburg University,Sweden*

Selectively growing carbon nanotubes requires an atomic scale understanding of the nanotube – catalyst particle interface, since this is the place where the carbon atoms incorporation takes place. According to recent experimental observations, the structure of the catalyst surface seems to be of importance. Using Density Functional Theory calculations [1], we calculate the structure of the interface and adhesion energies of carbon tubes on small particles of pure nickel or nickel carbide. The junctions between single-walled carbon nanotubes and nickel clusters are on the cluster surface, and not at subsurface sites, irrespective of the nanotube chirality, temperature, and whether the docking is gentle or forced. Gentle docking helps to preserve the pristine structure of the SWNT at the metal interface, whereas forced docking may partially dissolve the SWNT in the cluster. We then use these results to fine tune a tight binding model[2,3], which makes it possible to further investigate the effect of the temperature, chirality and particle size. [1] A. Börjesson et al, Nano Lett. 9, 1117 (2009) [2] H. Amara et al, PRB 79, 014109 (2009) [3] H. Amara et al, PRL 100, 056105 (2008)

### Dynamic superlubricity of graphene flake on graphite surface

**Irina Lebedeva**, *Moscow Institute of Physics and Technology, Russia; RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Russia* **Andrey Knizhnik**, *RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Russia* | **Andrey Popov**, *Institute of Spectroscopy, Russia* | **Olga Ershova**, *Moscow Institute of Physics and Technology, Russia* | **Yurii Lozovik**, *Institute of Spectroscopy, Russia* | **Boris Potapkin**, *RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Russia*

Different mechanisms of diffusion and drift of a graphene flake on a graphite surface are systematically analyzed using ab initio calculations and calculations with empirical potentials. A new mechanism of diffusion, “dynamic superlubricity”, is proposed. According to the proposed mechanism, rotational transition of the flake to incommensurate states takes place with subsequent simultaneous rotation and translational motion until the commensurate state is reached again, and so on. Due to the significant barrier for rotation of the flake, these events are rare. However, this factor is compensated by long distances passed by the flake before it returns to the commensurate state. The molecular dynamics simulations demonstrate that the proposed diffusion mechanism can be dominant under certain conditions. According to analytic expressions derived for the diffusion coefficient and mobility of the flake, the relative contribution of rotation to incommensurate states should be the most significant at temperature associated with the barrier for transition of the flake between adjacent energy minima in the commensurate state and should correspond to an increase of the diffusion coefficient by more than an order of magnitude. The results obtained can be also useful for study of dynamics of polyaromatic molecules on a graphite surface and should be qualitatively valid for a set of commensurate adsorbate-adsorbent systems. The methods of control over the diffusion and drift of graphene components in nanoelectromechanical systems are discussed. Moreover, the possibility to experimentally measure the barriers to relative motion of graphene layers by study of a graphene flake diffusion is considered.

### Curvature Effects on Optical Transitions in Semiconducting Carbon Nanotubes with Small Diameters

**Saloome Motavas**, *Department of Electrical and Computer Engineering, University of British Columbia* | **Andre Ivanov**, *Department of Electrical and Computer Engineering, University of British Columbia* | **Alireza Nojeh**, *Department of Electrical and Computer Engineering, University of British Columbia*

Due to their unique physical and electronic properties, carbon nanotubes are attractive candidates for optoelectronic and nanophotonic applications. Curvature and rehybridization strongly affect the electronic structure of small-diameter nanotubes and, as a consequence, have important implications on their optical properties. Here, we use first-principles/density functional theory calculations to study the curvature effects on the optical transitions in a number of semiconducting zigzag nanotubes with progressively smaller diameters, down to (4,0) nanotubes. We investigate the optical transition dipole moments and absorption rates for all possible transitions between various pi and sigma bands (including pi-sigma transitions) and the corresponding selection rules. We also examine how curvature affects the polarization dependence of light absorption. Various polarization angles ranging from parallel to perpendicular to the nanotube axis are considered. In general, for transitions from each valence sub-band, we observe that the parallel component of the dipole is a few times to an order of magnitude larger than that of the perpendicular component. Some exceptions exist; however, these usually correspond to large photon energies, leading to a low corresponding transition rate. For example, for an (8,0) nanotube, we show that the overall transition rate spectrum for perpendicular-polarized light is suppressed noticeably compared to the one for the parallel polarization of light. The relative strength of the parallel component of the dipole moment becomes stronger as the nanotube diameter decreases. To further investigate the curvature effects, we compare the results with those predicted using the conventional, pi-orbital tight-binding calculations within the zone-folding scheme.

### Mechanism study of gas phase floating catalyst synthesis of N-doped SWCNTs

**Toma Susi**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland* | **Giorgio Lanzani,** *Thule Institute, University of Oulu, Finland* | **Albert Nasibulin**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland* | **Paola Ayala**, *Department of Physics, University of Vienna, Austria* | **Tao Jiang**, *Department of Physics, Center for Atomic Scale Materials Design, Technical University of Denmark* | **Thomas Bligaard,** *Department of Physics, Center for Atomic Scale Materials Design, Technical University of Denmark* | **Kari Laasonen**, *Department of Chemistry, University of Oulu, Finland* | **Esko Kauppinen**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland*

We will present a gas phase floating catalyst method to synthesize N-doped SWCNTs in a simple continuous process using a hot iron wire/CO/ammonia system. In this method, the nanotube growth occurs on floating iron catalyst particles, with relatively simple chemistry involving CO, H2 and NH3 molecules. To study the mechanisms of doping, spin-polarized periodic density functional theory (GPAW code) was employed. In detail, the bonding and chemistry of CO, NH3 and their fragments on a Fe55 icosahedral cluster was considered. For NH3 adsorption, only the perpendicular N-interaction at the cluster is favorable (-0.73 eV < B.E.(NH3) < -0.53 eV), in agreement with recent experimental studies. Possible dissociation paths for NH3 to atomic nitrogen and hydrogen were identified. The calculated lowest reaction barrier for the overall process is comparable to an experimentally determined value (0.45 eV), obtained via FTIR and mass spectrometer measurements. For CO, only the perpendicular C-interaction is favorable. Dissociation occurs on a vertex between the facets, and while O atoms remain on the surface, C atoms move into the cluster as the initial step toward carbide formation. The CO dissociation barrier (0.63 eV) is lower than on most studied Fe surfaces. Several possible paths for C-C and C-N bond formation were also identified and found to be barrierless. A formation path for a secondary parasitic reaction producing HCN was identified, with a barrier of 1.65 eV, again in good agreement with the measured value (1.51 eV).

### Quantum Transport in Carbon Nanotubes and Graphene Based Materials: Localization Phenomena and Decoherence Effects

**Stephan Roche,** *Cea*

Graphene is a two-dimensional monolayer of $sp^2$ bonded carbon atoms in a dense honeycomb crystal structure which behaves electronically as a zero-gap semiconductor with exceptional chare mobilities. However the engineering of innovative devices demand for the extensive use of chemical treatment to clean or functionalize the raw material. This talk will overview some salient features of charge transport properties in chemically-doped or functionalized graphene based materials, with first the consideration of two-dimensional disordered graphene. In agreement with the 2D localization theory, the system will be shown to undergo a conventional 2D Anderson transition in the low temperature limit, providing inter-valley scattering processes are allowed, or say differently provided the material is sufficiently damaged. The sensitivity of localization phenomena in regards to edge symmetries and change of transport dimensionality or disorder scale will be further outlined. The effect of chemical disorder, including Boron and Nitrogen substitutions, topological defects, vacancies and grafted molecules will be also discussed. Chemical modifications of graphene material will be demonstrated to strongly impact on electronic properties of graphene. We will also discuss the limits of coherent transport, considering the effect of electron-phonon interaction on quantum interferences phenomena, as well as the onset of decoherence effects.

### Charge Transport in Carbon-based Materials At The Mesoscopic Scale

**Alejandro Lopez Bezanilla**, *Oak Ridge National Laboratory*

I will present a theoretical methodology to explore conduction regimes through micrometer long systems within a fully ab initio approach, by resorting to both first principles calculations and the Green function formalism applied to the Landauer transport approach. Charge quantum transport through graphene nanoribbons and carbon nanotubes with randomly distributed functional groups covalently attached to the system surface is analysed. Phenyls and hydroxyl groups induce a sp2 to sp3 local orbital rehybridization of the anchor carbon atoms yielding to the localized transport regime. On the other hand, carbene functional groups do not disrupt the original hyperconjugated network of armchair and small diameter zigzag nanotubes which allows for good conductance preservation.

# 6th International Symposium on Computational Challenges and Tools for Nanotubes 2010 (CCTN10)

## ROOM: OUTREMONT

## Monday, June 28

### ■ *Mechanical Chemistry*

### 8:40-9:20 Invited Speaker

**Helical Nanotube Structures with Intrinsic Twisting: An Objective Molecular Dynamics Study**
**Traian Dumitrica**, Univ. Of Minnesota, USA

Understanding the interplay between the ionic and electronic degrees of freedom in chiral nanostructures is of fundamental importance. Unfortunately, the properties of chiral nanotubes (NTs) are less investigated, partially due to the inconvenience of handling chirality within the standard treatments of crystalline solids. Objective molecular dynamics (MD) [1] is a recent generalization of MD to helical boundary conditions. The approach allows computing chiral NTs due to an introduced simplification in the number of atoms that need to be accounted for. Using it coupled with extended density functional theory-based nonorthogonal tight binding, we compute NTs in a nanomechanical way, as the result of the Eshelby's twist introduced by the axial screw dislocation. New findings often come by using new investigation methods. We reveal that chiral molybdenum disulphide (MoS2) NTs store an intrinsic twist [2] that removes the translational symmetry and makes the standard treatments inapplicable. Fortunately, the helical symmetry introduced by the Eshelby's twist combined with objective MD provide the suitable theoretical framework to investigate properties. We find that MoS2 NTs have chirality-dependent fundamental band gaps and elastic responses. The possibility of intrinsic twist in carbon and boron nitride nanotubes will be addressed. [1] T. Dumitrica and R.D. James, Objective Molecular Dynamics, Journal of the Mechanics and Physics of Solids 55, 2237 (2007). [2] D.-B. Zhang, T. Dumitrica, and G. Seifert, Helical Nanotube Structures of MoS2 with Intrinsic Twisting, Physical Review Letters 104, 065502 (2010).

### 9:20-9:40 Contributed Talk

**Collapse of carbon nanotubes: a comparison of theory with atomistic simulations**
**James Elliott**, *University Of Cambridge, United Kingdom* | **Juan Vilatela**, *University Of Cambridge, United Kingdom* | **Nicola Pugno**, *Polytechnic of Turin* | **Alan Windle**, *University Of Cambridge, United Kingdom*

We present a theory for predicting the critical radius for the self-collapse of carbon nanotubes in a bundle, and relate this to previous molecular dynamics simulations of single, double and multi-wall nanotube bundles under hydrostatic pressure [1]. The results show good agreement with experimental high-resolution electron micrographs [2] from nanotubes in carbon nanotube fibres produced by the Cambridge fibre spinning process [3]. These show bundles containing nanotubes with a range of geometries ranging from cylindrical to fully collapsed, depending on diameter and number of walls. The collapse transition in carbon nanotube bundles is rationalized by a balance between the interfacial cohesive energy between tubes and their elastic strain energy. We discuss the implications for stress transfer between nanotubes in bundles in the context of improving mechanical properties of macroscopic assemblies of nanotubes. [1] J. A. Elliott, J. K. W. Sandler, A. H. Windle, R. J. Young, and M. S. P. Shaffer, Physical Review Letters 92 (9) (2004). [2] M. Motta, A. Moisala, I. A. Kinloch, and A. H. Windle, Advanced Materials 19, 3721 (2007). [3] Y. L. Li, I. A. Kinloch, and A. H. Windle, Science 304 (5668), 276 (2004).

### 9:40-10:00 Contributed Talk

**Bromophenyl functionalization of carbon nanotubes using the ONETEP code**
**Jason Beaudin**, *Département de physique, Université de Montréal, Canada* | **Jonathan Laflamme Janssen,** *Département de physique, Université de Montréal, Canada* | **Michel Côté**, *Département de physique, Université de Montréal, Canada* | **Peter D. Haynes,** *Département de physique, Université de Montréal, Canada*

One of the main research efforts of the recent years has been the development of an efficient way to select desired carbon nanotubes according to their size and their electronic properties. This selectivity would allow easier fabrication of field effect transistor and light-emitting diode devices with appropriate nanotubes. An appealing approach to address this problem is to establish the rules of chemical functionalization of this material. In this talk, I will present ab initio calculations of carbon nanotubes functionalized with bromophenyl. I will report the radius dependance of the binding and activation energies of this functionalization. The purpose of this presentation is also to demonstrate the use of the linear-scaling density-functional code ONETEP which uses nonorthogonal generalized Wannier functions, providing the possibility of large system calculations up to several hundreds of atoms.

### Coffee Break

### ■ *Charge Transport*

### 10:30-11:10 Invited Speaker

**First principles modelling of spin polarised transport in carbon nanostructures**
**Jesse Maassen**, *Centre for the Physics of Materials and Department of Physics, McGill University, Canada* | **Youqi Ke**, *Centre for the Physics of Materials and Department of Physics, McGill University, Canada* | **Zi Wang**, *Centre for the Physics of Materials and Department of Physics, McGill University, Canada* | **Wei Ji**, *Centre for the Physics of Materials and Department of Physics, McGill University, Canada* | **Hong Guo,** *Centre for the Physics of Materials and Department of Physics, McGill University, Canada*

We report a first principles theory for calculating quantum transport properties of nanostructures with atomistic disorder. The theory is based on the non-equilibrium vertex correction (NVC) to handle the configurational average of random disorder at the density matrix level. Combined with the Keldysh nonequilibrium Green's function (NEGF) and density functional theory (DFT), disorder effects to nonlinear and non-equilibrium quantum transport can be calculated in a self-consistent manner. We will report our investigations of spin polarised quantum transport in several carbon nanostructures including graphene and graphene nano-ribbons.

### 11:10-11:50 Invited Speaker

**Large-scale Simulation on Electron Conduction in Carbon Nanotubes at Finite Temperature**
**Satoshi Nakamura**, *Research Organization For Imfomation Science And Technology, United Kingdom* | **Syogo Tejima**, *Research Organization For Imfomation Science And Technology, United Kingdom* | **Mikio Iizuka**, *Research Organization For Imfomation Science And Technology, United Kingdom* | **Hisashi Nakamura**, *Research Organization For Imfomation Science And Technology, United Kingdom* | **David Tomanek**, *Department of Physics and Astronomy, Michigan State University*

Carbon nanotubes are expected to be applied to electronic devices due to their unique properties. Some devices such as random access memory and radio receiver have already been developed up to a considerable stage. In order to fully achieve control on the properties of carbon nanotube-based devices, it is important to perform analyses of the carbon nanotubes of which the sizes are the same as those observed in experiments in meso-scale. We propose an advanced tight-binding molecular dynamical (TBMD) method that can treat the time-dependent electromagnetic field and the retardation of electron response to lattice motion, by implementing the non-equilibrium Greenfs function (NEGF) method for calculating the electron-conduction in carbon nanotube that is connected to the electrodes at finite bias voltages and temperature. The NEGF in the scattering region, which becomes the heaviest part of the computational load in this method, is calculated by adopting an embedding potential algorithm. Our results show that the advanced TBMD code developed by us makes it possible to perform large-scale simulations with linear system-size, i.e., order-N simulations.

### Lunch

## ■ *Atomistic view*

### 13:40-14:20 Invited Speaker

**Forces and Currents in FM-AFM Experiments on Low-dimensional Carbon Materials: Are we imaging atoms?**

**Rubén Perez**, *Universidad Autonoma De Madrid, Spain*

In spite of the apparent simplicity of the structure common to fullerenes, nanotubes and graphene --Graphite can be imaged with atomic resolution with STM even in ambient conditions-- and the long-time experimental research effort combining STM and AFM, there is an ongoing controversy regarding the origin of the atomic contrast: we do not know yet if the maxima on the SPM images correspond to atoms or to the hollow sites. In this work, we assess this problem with a study that combines DFT total-energy calculations with Non-equilibrium Green's Function (NEGF) methods for electronic transport in order to determine the interaction and the tunneling current [1,2] between a large set of AFM tips with different low-dimensional carbon materials. We have considered several possible tip terminations: reactive clean Si tip apexes, non-reactive apexes, oxygen contaminated Si apexes and metallic tips. Our calculations show that (1) the observed bright protrusions in FM-AFM experiments correspond to either atoms or hollow sites depending on the tip reactivity; and (2) the vdW interaction may contribute significantly to the total attractive force (particularly for the less reactive tips) but does not provide any atomic-scale contrast, that comes entirely from the Pauli repulsion in the short-range chemical interaction. Finally, we analyze the tunneling currents as a function of the tip-sample distance and identify the conditions for contrast reversal in STM. [1] Y. Sugimoto et al., Nature 440, 46 (2007). [2] P. Jelinek et al., Phys. Rev. Lett. 101, 176101 (2008).

### 14:20-14:40 Contributed Talk

**Understanding the Nucleation Mechanisms of Carbon Nanotubes in Catalytic Chemical Vapor Deposition**

**Hakim Amara**, *Laboratoire d'Etude des MIcrostructures, Onera-Cnrs, France* | **Christophe Bichara**, *CINaM, CNRS, Marseille, France* | **François Ducastelle**, *Laboratoire d'Etude des MIcrostructures, Onera-Cnrs, France*

Although MWNTs are now produced on an industrial scale, a detailed understanding of the synthesis mechanisms of SWNTs is still mandatory for more elaborate applications. Indeed, simple questions such as the role and physical state of the catalyst are still not answered. Remarkable progress has been made in the in situ observation of the growth, but the atomic resolution is not yet obtained under these conditions. Computer simulation is then a unique tool to gain insight at this atomic scale that is very difficult to access experimentally. In this work, we adopt a new approach, using a tight binding model for Ni-C interactions coupled to grand canonical Monte Carlo simulations, to gain a new insight on the nucleation of carbon caps on small nickel clusters [1]. We have shown that optimal conditions exist to nucleate nanotube caps whose curvature match the local curvature of the catalyst particle. The nucleation is triggered when the concentration of C atoms adsorbed on the surface is large enough.The role of the catalyst is to conne C atoms on or close to the surface, and to make them reach this critical concentration [2]. [1] H. Amara et al, PRB 79, 014109 (2009) [1] H. Amara et al, PRL 100, 056105 (2008)

### 14:40-15:00 Contributed Talk

**Early Stages in the Nucleation Process of Carbon Nanotubes: Density-Functional Tight-Binding Molecular Dynamics Simulations of Acetylene Oligomerization and Cross-Linking on an Fe38 Particle**

**Ying Wang**, *Institute for Advanced Research and Department of Chemistry, Nagoya University, Japan* | **Yasuhito Ohta**, *Department of Chemistry Faculty of Science, Nara Women University, Japan* | **Hu-Jun Qian**, *Institute for Advanced Research and Department of Chemistry, Nagoya University, Japan* | **Stephan Irle**, *Department of Chemistry Faculty of Science, Nara Women University, Japan* | **Keiji Morokuma**, *Fukui Institute for Fundamental Chemistry, Kyoto University, Japan*

Catalytic chemical vapor deposition (CCVD) is typically used to synthesize carbon nanotubes (CNTs), but the exact role of metal catalysts is still unknown. Since Fe substrate is known to be highly effective for the CNT growth in the CCVD process and C2H2 is the major decomposition product from feed hydrocarbons, we performed quantum chemical molecular dynamics (QM/MD) simulations based on the density-functional tight-binding (DFTB) method to investigate self-assembly of carbon nanotubes from acetylene on an Fe38 particle. We report oligomerization and cross-linking reactions as initial steps toward cap nucleation. We found during 30 ps simulations under continued acetylene supply that H may occasionally transfer to the iron particle or other C2H2 to form C2Hx species. Subsequently, these more reactive species initiate oligomerization reactions. During extended 80 ps carbon diffusion simulations, five or six-membered rings as well as longer carbon chains were formed, indicating cross-linking of polyacetylene-like chains. Accompanying our QM/MD simulations, we computed the barrier heights for four kinds of reactions at the DFTB level: H-transfer (~40 kcal/mol), C-C bond breaking (~45 kcal/mol), H2 abstraction (~70 kcal/mol), and C-C oligomerization (~23 kcal/mol). Although only a limited number of structures was systematically investigated this way, the MD simulations confirm that C-C oligomerization occurs readily since it is an exothermic reaction (~ -10 kcal/mol). To the contrary, H2 abstraction possesses a very high barrier and is an endothermic process (~68 kcal/mol), and was consequently never observed in MD.

### Coffee Break

## ■ *Complex NT Materials*

### 15:30-16:10 Invited Speaker

**Theoretical and Computational Modeling of Carbon-Based Supercapacitors**

**Vincent Meunier**, *Oak Ridge National Laboratory, USA* | **Jingsong Huang**, *Oak Ridge National Laboratory, USA* | **Bobby Sumpter**, *Oak Ridge National Laboratory, USA* | **Guang Feng**, *Clemson University* | **Rui Qiao**, *Clemson University*

Theoretical methods have evolved to a point where the properties of materials can be successfully predicted based solely on their atomic structure. As such, they provide a unique tool, able to help identifying the origins of the properties of a given structure and uncovering principles that can be used to tailor structure for target applications. In this talk, I will present an overview of the theoretical and computational work we have recently performed on capacitive electrical energy storage [1-5]. I will present a new heuristic model that avoids the shortcomings of the electrical double-layer capacitor (EDLC) model by considering explicitly pore curvature. The density functional theory based model explains experimental observations for a range of pore sizes: from the micropore regime (< 2 nm), mesopore regime (2-50 nm), and macropore regime (> 50 nm); and diverse carbon materials and electrolytes. The model allows the properties of a supercapacitor to be correlated with pore size, specific surface area, Debye length, electrolyte concentration, dielectric constant, and solute ion size, and lead to a optimization pathway of carbon supercapacitors properties through experiments. I will also present our recent findings on the ion dynamics and its effect on capacitor performance [3-4] as well as a new paradigm for exhohedral capacitors [5]. References: [1] Angewandte Chemie 47, 520 (2008). [2] Chemistry: A European Journal (CEJ), 14, 6014 (2008). [3] Microfluidics and Nanofluidics, in press (2010); [4] Phys. Chem. Chem. Phys., 2010, DOI:10.1039/ (in press), (2010) [5] J. Mat. Res., in press, (2010)

## 16:10-16:30 Contributed Talk

### Mechanical, electronic and transport properties of carbon nanotubes in a cross structure

**Ali Kashefian Naieni**, *Department of Electrical and Computer Engineering, University Of British Columbia, Canada* | **Parham Yaghoobi**, *Department of Electrical and Computer Engineering, University Of British Columbia, Canada* | **Alireza Nojeh**, *Department of Electrical and Computer Engineering, University Of British Columbia, Canada*

Due to their quasi one-dimensional nature, nanotubes are ideal candidates for making quantum devices. A nanotube cross is a structure made by a carbon nanotube passing over another one at an angle. Because of the induced mechanical deformation at the intersection point, the electronic properties of the nanotubes in a cross could vary significantly from those of intact nanotubes, potentially leading to the formation of nanoscale quantum dots. We report a theoretical study of the mechanical, electronic and transport properties of semiconducting and metallic nanotubes in a cross structure. Physically viable and stable configurations were found using molecular dynamics simulations. It was observed that the final configuration the nanotube relaxes to does not depend strongly on the initial guess for its shape. The electronic structure of the most deformed part of the top nanotube in the cross was then found using first-principles calculations. Band gap change as a result of deformation was observed in tubes with various chiralities and different degrees of deformation. The current-voltage characteristics of the deformed nanotubes were then calculated using a transport solver developed in-house. This code uses the results of the first-principles simulations of the electronic structure in a nonequilibrium Green's function formalism with a three–dimensional, real-space basis. The transmission probability of electrons through the deformed nanotubes as a function of applied voltage is calculated and the total current obtained through the Landauer-Buttiker formula. The changes in the transport characteristics of different carbon nanotubes with various levels of deformations are discussed.

## 16:30-16:50 Contributed Talk

### A new first-principles junction model based on capped carbon nanotubes

**Yong-Hoon Kim**, *University Of Seoul, Korean Republic* | **Ga In Lee**, *Korea Advanced Institute of Science and Technology* | **Jeung Ku Kang**, *Korea Advanced Institute of Science and Technology*

One of the key challenges for the first-principles study of carbon nanotube (CNT)-metal contacts has been the limitations of the two representative atomistic contact models, open-ended and side-contacted junctions, in capturing the experimental situations. We here propose a new junction models based on capped (10,0) CNTs, which enables us to systematically investigate the charge injection process acroos metal-CNT contacts. Applying a fully converged first-principles calcualtion approach [1], we analyze the atomic structure, level alignment, decay behavior of metal-induced gap states, and charge injection properties of the junction models, and most importantly demonstrate the intrinsic difficulty of constructing reliable (with a consistent device type) high-performce (based on strong contacts) CNT devices. Comparison with the previous studies based on more approximate computational schemes will also be discussed. [1] Y.-H. Kim, S. S. Jang, Y. H. Jang and W. A. Goddard III, Phys. Rev. Lett. 94, 156801 (2005); Y.-H. Kim and Y. M. Byun, J. Kor. Phys. Soc. 55, 299 (2009)

## 16:50-17:00

### CCTN10 Committee, Closing Remarks

## 18:00-20:00

### NT10 Welcome Reception

# 4th International Workshop on Metrology, Standardization and Industrial Quality of Nanotubes (MSIN10)

**Organizers:**
**Ken Bosnick**, *National Institute for Nanotechnology, National Research Council Canada*
**Jennifer Decker**, *National Institute of Measurement Standards, National Research Council Canada*
**Mildred Dresselhaus**, *Department of Electrical Engineering & Computer Science and Department of Physics, MIT, USA*
**Ado Jorio**, *Departamento de Física, Universidade Federal de Minas Gerais, Brazil*
**Chris Kingston**, *Steacie Institute for Molecular Sciences, National Research Council Canada*

## ROOM: VERDUN

## Sunday, June 27

### 8:30

**Call to Order & Welcome**
**Alan Steele**, *National Research Council Canada*

## ■ *Session: Chemical Metrology*

**(Chair: Alan Steele)**

### 8:40 Invited Speaker

**Carbon nanomaterials, a showcase for standardised characterisation**

**Nicole Grobert**, *University Of Oxford, United Kingdom* | **Antal A Koos**, *University Of Oxford, United Kingdom* | **Irene Suarez-Martinez**, *IMN, Universite de Nantes; Curtin University of Technology* | **Frank Dillon**, *University Of Oxford, United Kingdom* | **Zabeada Aslam**, *University Of Oxford, United Kingdom* | **Geoffrey Otieno**, *University Of Oxford, United Kingdom* | **Andrew Searle**, *University Of Oxford, United Kingdom* | **Jingyu Sun**, *University Of Oxford, United Kingdom* | **Adrian Murdock**, *University Of Oxford, United Kingdom* | **Fatma Dinc**, *University Of Oxford, United Kingdom* | **Madhuri Dutta**, *University Of Oxford, United Kingdom* | **Sarah Downes**, *University Of Oxford, United Kingdom* | **Teodor-Matei Cirstea**, *University Of Oxford, United Kingdom* | **Christopher P Ewels**, *IMN, Universite de Nantes* | **Alison Crossley**, *University Of Oxford, United Kingdom*

The rapid development of nanomaterials and more specifically carbon nanomaterials brings an urgent need for a systematic characterisation protocol as well as standardised nomenclature. Following the initial gold rush identifying new carbon nanoforms, the field is slowly maturing. Attempts are now being made to systematically reproduce and isolate specific carbon nanoforms. Carbon nanostructures range from structurally well defined molecules such as fullerenes to larger 'macromolecules' for which the atomic arrangement can not be stoichiometrically precisely defined. Therefore, conventional IUPAC chemical notation is insufficient. Here, we propose a nomenclature based on the morphology which is sufficiently general to conveniently group materials, while remaining specific enough to describe local structural variations. Furthermore, establishing a rigorous characterisation protocol is rather complex and not very straight forward and hence still not widely distributed or in fact applied. Therefore, we will high-light a few, very simple, procedures that do not rely on the use of state-of-the-art characterisation tools but that can be carried out with equipment available in most laboratories. Taking into account the complexitiy of the problem as such, it is important to establish an inclusive approach to a standardised characterisation protocol, e.g. the more reseach groups are able to follow the protocol the easier it is to get it ingrained in on-going research activities, and therefore paving the way to better classification procedures for nanomaterials.

### 9:10 Invited Speaker

**Metrology of Defects in Graphitic Materials: Challenges and Implications for Developing New Nano-Devices**
**Mauricio Terrones**, *University Carlos III Of Madrid, Spain*

Different types of defects within graphene and carbon nanotubes: 1) Structural defects; 2) Bond rotations or grain boundaries; 3) Doping-induced defects; 4) Non-sp2 carbon defects or edge-sites, and 5) Folded (or highly strained) graphene. We will review different techniques used to identify defects: SEM, HRTEM, STM, STS, AFM, Raman spectroscopy (RS), photoluminescence spectroscopy (PLS), thermogravimetric analyses (TGA), electron and thermal transport measurements, etc. The presence of defects and their identification has been overlooked by numerous scientists. However these play a key role in the nanotubes' physico-chemical properties and even biocompatibility. We will answer the following questions: 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 3D architectures? Could I introduce specific defects in order to make materials biocompatible? Could we promote ferromagnetism by introducing specific defects in nanostructures? Could I control their specific reactivity in order to use them as sensors, filters or drug deliverers? etc.

### 9:40 Contributed Talk

**Characterization of the dispersability of different carbon nanotube materials**
**Beate Krause**, *Leibniz Institute of Polymer Research Dresden, Germany* | **Mandy Mende**, *Leibniz Institute of Polymer Research Dresden, Germany* | **Gudrun Petzold**, *Leibniz Institute of Polymer Research Dresden, Germany* | **Petra Pötschke**, *Leibniz Institute of Polymer Research Dresden, Germany*

For the effective use of carbon nanotubes (CNT) excellent distribution and dispersion are essential preconditions. Among the parameters determining the dispersion the dispersability of the CNT materials is of main influence. This quality was assessed studying the sedimentation behavior of CNT under centrifugal forces dispersed in aqueous surfactant solutions at different ultrasonication treatment times using a LumiSizer® apparatus. Different industrial available multiwalled CNT, namely Baytubes® C150P, Nanocyl® NC7000, Arkema Graphistrength® C100, and FutureCarbon CNT-MW showing quite different kinetics were compared. In addition, the particle size distributions were analyzed using dynamic light scattering (DLS, ZetaSizer) and centrifugal separation analysis (CSA). The best dispersability was found for Nanocyl® NC7000 and FutureCarbon CNT-MW. To prepare stable dispersions of Baytubes® C150P and Graphistrength® C100 five times more energy input was necessary. These finding correlates with the values of deformation stress measurements on the primary agglomerates which resulted in lower values for Nanocyl® NC7000 than for Baytubes® C150P and Graphistrength® C100. In addition, the higher deformation stress of Baytubes® C150P and Graphistrength® C100 is in good agreement with the higher bulk densities of 120-170 and 50-150 kg/m3, respectively. In contrast, Nanocyl® CNT having a low bulk density of 66 kg/m3 exhibits also a lower deformation stress value. The size of the primary agglomerates in the dry nanotubes powder as evidenced by SEM investigations and laser light diffraction measurements was found not to influence the dispersability. These results help to optimize the processing of nanocomposites depending on the applied carbon nanotube materials.

### 10:00 Break

## ■ *Session: Standards*

**(Chair: Clive Willis)**

## 10:10 Invited Speaker

### Developing an international standard on terminology for carbon nano-objects

**Shuji Abe**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan*

Given the importance of carbon nanomaterials in nanotechnologies, ISO/TC 229 and IEC/TC 113 Joint Working Group 1 (Terminology and Nomenclature) has been developing a technical specification (TS) on vocabulary for carbon nano-objects, which will be published as Part 3 of the TS 80004 series [1]. The most important aspect of this work is harmonization with a rational hierarchical system of terminology under development for nanotechnologies. This means, for example, the definition of 'carbon nanotube' must follow the definition of the parent term 'nanotube'. However, in some cases the hierarchical approach needs to be compromised due to the specific usage of individual terms or due to the limited scientific knowledge of material characteristics. The evolution and future directions on terminology and nomenclature for carbon nanomaterials will be discussed.
[1] ISO TS 80004-3: 2010, Nanotechnologies -- Vocabulary -- Part 3: Carbon nano-objects.

## 10:40 Invited Speaker

### Documentary Standards Development for Carbon Nanotube Characterization within ISO/TC 229

**Angela Hight Walker**, *National Institute Of Standards and Technology, USA*

Carbon nanotubes (CNTs) play a prominent role within the International Standards Organization (ISO), Technical Committee (TC) 229 Nanotechnology. ISO/TC229, established in 2005, has 32 member body countries participating and 10 countries observing, and works in cooperation with multiple organizations such as CEN, OECD, VAMAS, Asia Nano Forum, BIPM, IUPAC among others. CNTs are the focus of the vast majority of work items within Working Group 2 (WG2), Measurement and Characterization, one of the four WGs within the TC. WG2 is a joint committee with the International Electrotechnical Commission (IEC)/TC 113. The work program for single-wall carbon nanotubes is based on a matrix of six parameters verses multiple measurement methods. Many of these technique-based projects have moved into the final stages of development. Also, multiwall carbon nanotube characterization is under consideration within WG2. A summary of the documentary standards under development pertaining to carbon nanotubes will be presented, particularly those within ISO/TC229, but also those relevant activities in other standards developing organizations.

## 11:10 Invited Speaker

### Scanning probe microscopy standardization using and for measurement of carbon nanotubes

**Charles Clifford**, *National Physical Laboratory, United Kingdom*

Scanning probe microscopy (SPM) family are powerful instruments that can give dimensional, mechanical, electrical and some chemical information at the nanoscale and are thus ideally suited to studying carbon nanotubes. In 2004, international standardisation of SPM methods began with the creation of a sub-committee on scanning probe microscopy in ISO/TC 201 on surface chemical analysis. In this talk, we highlight the work that is being undertaken in this technical committee with several examples that are being led by NPL. The first is a draft ISO standard on methods to calibrate AFM normal spring constants, necessary to give quantified force. The second is terminology, which include 76 SPM acronyms, 33 definitions of SPM techniques, 6 terms for contact mechanics and 147 SPM terms. The talk will also highlight research being undertaken at NPL analyzing carbon nanotubes using various SPM techniques. These include using carbon nanotubes and other samples to determine the AFM tip shape. This is critical for high resolution, accurate dimensional measurements. Tip enhanced Raman spectroscopy (TERS) is also being used to characterize carbon nanotubes to give some chemical information at the nanoscale. Methods to assess dispersions of carbon nanotubes are also being investigated.

## 11:40 Contributed Talk

### Measurement vs. Metrology

**Jennifer Decker**, *National Research Council Canada - Institute For National Measurement Standards, Canada* | **Alan Steele**

Metrology forms the bridge from science to technology. Precise knowledge of characteristics such as traceability, measurement uncertainty, reproducibility, repeatability is what differentiates one single measurement observation from a metrological measurement. Metrology differs somewhat from measurement in the manner of scope. Traceability to a single reference means that all measurements can be compared with each other on a common scale. The SI system of units provides this global framework. Science continues to push on frontiers of knowledge, and the transformation of science into technology is underpinned by profound understanding and predictive models, which can only be attained via measurement results which are widely reliable and comparable. Reference materials provide a means to establish a base-line result with which to compare other materials measured the same way. Protocols for sample preparation [1] and measurement methods are important contributors to comparability. The content of such protocols is based on measurement repeatability within labs and duplication of results amongst peer labs. At this formative stage of our knowledge, independent demonstration of the same result validates measurement and uncertainty models and provides confidence in the robustness of a method. Statistical methods specifically targeted for comparing measurements have been developed [2]. This talk outlines these cornerstone concepts with some specific examples. 1. Decker, J.E., et al, 2009 "Sample Preparation Protocols for Realization of Reproducible Characterization of Single-Wall Carbon Nanotubes", Metrologia 46 (6), 682-692. 2. Decker, J.E., Steele, A.G., Douglas, R.J. 2008 'Measurement science and the linking of CIPM and regional key comparisons', Metrologia 45(2), 223-232.

## 12:00 Lunch

## ■ *Session: Physical Metrology*

**(Chair: Ado Jorio)**

## 13:00 Invited Speaker

### Single walled carbon nanotube material assessment using photoluminescence

**Jacques Lefebvre**, *National Research Council, Canada*

After the first report of fluorescence (or alternatively photoluminescence) in individualized micelle encapsulated single walled carbon nanotubes, the nanotube community has quickly recognized its potential as a powerful tool for materials assessment. I will describe with several examples taken from the literature how the method is currently being used, and highlight the important advances that greatly benefited from photoluminescence. As with every method, users ought to be aware of some fundamental issues setting the limitations of their characterization tool and this is more so true for photoluminescence. Nanotube luminescence is primarily a very active research topic and the findings might affect the conclusions of a sample analysis. I plan to give an overview of the current knowledge and how it impacts materials assessment. Finally, I will outline some important guidelines to users of photoluminescence as a characterization tool which are soon to be published as an ISO Technical Specification.

## 13:30 Invited Speaker

### Mechanism of Near-field Raman Enhancement in Carbon Nanotubes

**Luiz Gustavo Cancado**, *Departamento de Fisica, Universidade Federal de Minas Gerais, Brazil.* | **Ado Jorio**, *Departamento de Fisica, Universidade Federal de Minas Gerais, Brazil* | **Achim Hartschuh**, *Department Chemie und Biochemie and CeNS, Germany* | **Ariel Ismach**, *Department of Materials and Interfaces, Weizmann Institute of Science,Israel* | **Ernesto Joselevich**, *Department of Materials and Interfaces, Weizmann Institute of Science,Israel* | **Lukas Novotny**, *University of Rochester, The Institute of Optics, USA*

Many experimental works have recently shown that near-field Raman is an useful optical technique for the study of carbon nanotubes on the nanometric scale. The high-resolution achieved in these experiments (~10-30 nm) made it possible to resolve local variations in the Raman spectrum along an isolated single-wall carbon nanotube, which would otherwise be hidden in far field measurements. In spite of the great potential of near-field Raman on the development of the science of carbon nanotubes, a careful analysis taking in account its theoretical basis still missing. In this talk, we present a theory describing the near-field Raman enhancement of carbon nanotubes. The theory predicts that the near-field Raman intensity is inversely proportional to the 10th of the tip-sample distance. Supporting the theory, experimental results of near-field Raman measurements performed on distinct serpentines carbon nanotubes (with different chiralities) is presented. The experimental data show that distinct peaks present in the near-field Raman spectra originated from an specific tube present the same enhancement for a given tip-sample distance. These results indicate that the near-field enhancement does not dependent considerably on the symmetry of the Raman mode, but mainly on the field enhancement factor intrinsic from the near-field probe used in the experiment.

## 14:00 Contributed Talk

### The Role of Doping of Single-Walled Carbon Nanotubes in Metrology

**Martin Kalbac**, *J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Czech Republic.; Department of Electrical Engineering and Computer Science, USA* | **Hootan Farhat**, *Department of Materials Science and Engineering, MIT, USA* | **Ladislav Kavan**, *J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Czech Republic.* | **Jing Kong**, *Department of Electrical Engineering and Computer Science, USA* | **Ken-ichi Sasaki**, *National Institute for Material Science, Japan* | **Riichiro Saito,** *Department of Physics, Tohoku University, Japan* | **Mildred S. Dresselhaus**, *Department of Electrical Engineering and Computer Science, USA; Department of Physics, MIT, USA*

In the present work we discuss the influence of doping single-walled carbon nanotubes on their use in metrology, based on Raman spectroscopy. In this connection we have analyzed the radial breathing mode intensity vs. electrode potential profiles in the Raman spectra at many different laser excitation energies. It is shown that the charging of carbon nanotubes causes a broadening of the resonant Raman profiles and also give rise to a shift in energy of the resonance maximum. The change of the resonance profile has important practical consequences on the quantitative determination of the amount of a given (n,m) tube that is contained within a given nanotube sample. This is because the presence of carriers will have a different effect on the radial breathing mode intensity at different laser excitation energies. The effect of doping is in particular important in the case of metallic tubes. In contrast to semiconducting tubes, in the case of metallic tubes for which the laser is close to their maximum in the resonance profile, the Raman intensity is strongly bleached by natural doping, and thus the amount of these particular nanotubes present in a given sample when evaluated on the basis of a measurement of the radial breathing mode intensity might be strongly underestimated. Particular attention is given to analysis of their metrological effect.

## 14:20 - Contributed Talk

### X-ray diffraction as a tool for quantitative structural characterization of single-walled as well as multi-walled carbon nanotube batches

**Julien Cambedouzou**, *Laboratoire de Physique des Solides, France* | **Pascale Launois**, *Laboratoire de Physique des Solides, France*

Low-cost methods to characterize carbon nanotubes (CNT) are strongly needed in the context of their large-scale industrial production. Methods such as electron microscopy or Raman spectroscopy cannot be used easily in a quantitative way on macroscopic nanotube samples, due to the local character of the method in the first case and to resonance effects in the second case. X-ray diffraction (XRD) allows one to probe several milligrams of nanotube samples. Low-cost experiments can be performed on laboratory anodes, the use of synchrotron radiation being not necessary here. We will show that analysis of XRD data using adequate modeling of diffraction patterns gives access to key structural parameters of nanotube batches such as : (i) mean-diameter, distribution in diameters, organization in bundles if any, for single-walled (SW) CNT [1], (ii) number of walls, inter-wall distances and possible organization in bundles for multi-walled (MW) CNT [2]. Nano-contaminants (catalyst nanoparticles, graphitic shells, etc) are also probed by XRD. For macroscopic quantities of single helicity nanotubes, XRD would allow determination of the helicity. Moreover, preferential orientation of nanotubes, in composites for instance, are quantified using XRD [3]. We will present XRD diffraction patterns of SW, double-walled and MWCNT from several academic and industrial suppliers and we will discuss their structural characteristics. [1] G. Charron et al., New J. Chem. 33, 1211 (2009) [2] J. Cambedouzou et al., Phys. Rev. B 79, 195423 (2009) [3] V. Pichot et al., Phys. Rev. B 74, 245416 (2006)

## 14:40 Contributed Talk

### Voltage-contrast scanning electron microscopy for statistical analysis of metallic and semiconducting SWNT devices and location and characterization of defects

**Aravind Vijayaraghavan**, *Massachusetts Institute Of Technology, USA; Karlsruhe Institute of Technology* | **Ralph Krupke**, *Karlsruhe Institute of Technology*

Single-wall carbon nanotubes (SWNTs) are edging closer to electronic applications, with successful techniques now available for sorting and large-scale integration. When SWNTs are integrated into arrays or circuits at high densities, it is required to characterize the number and location of metallic and semiconducting devices among them. This is true even when such arrays are assembled using high-purity semiconducting SWNT solutions since it becomes critical to locate stray metallic devices that would significantly affect overall performance. Here, we describe voltage-contrast scanning electron microscopy (VC-SEM), as a fast, user-friendly and non-invasive technique for the simultaneous electronic characterization of arrays of SWNTs devices. We demonstrate how metallic and semiconducting SWNTs can be distinguished in an SEM under the influence of a substrate bias, and describe the underlying mechanism. In addition, devices containing SWNTs with defects can also be identified. On closer inspection, we can reveal the location and nature of such defects with nano-scale resolution (Featured on cover of Carbon 48(4)). Anomalies such as charge-injection into the substrate which leads to hysteresis, as well as in-situ characterization of the creation and annealing of defects (defect engineering) will also be demonstrated using VC-SEM. Vijayaraghavan, A., et al., Imaging defects and junctions in single-walled carbon nanotubes by voltage-contrast scanning electron microscopy, Carbon 2010, 48(2), 494 Vijayaraghavan, A.; et al., Imaging electronic structure of carbon nanotubes by voltage-contrast scanning electron microscopy. Nano Research 2008, 1, 321 Vijayaraghavan, A.; et al., Ultra-Large Scale Directed Assembly of Single-Walled Carbon Nanotube Devices. Nano Letters 2007, 7, 1556-1560.

## 15:00 Break

## ■ *Session: Graphene*

**(Chair: Ken Bosnick)**

### 15:15 Invited Speaker

**Overview of the metrology of graphene**

**Alain Diebold**, *College Of Nanoscale Science And Engineering, USA*

Graphene is considered a strong candidate for extending transistor technology and as a material for beyond CMOS switches. New materials such as graphene are difficult to find, manipulate, and measure. Chemical Vapor Deposition and annealing of SiC wafers both may provide the large area graphene necessary for device manufacturing. There are many questions about how to compare the many physical and electrical measurements and evaluate new growth methods. This talk will discuss many of the key measurement areas. The electrical properties of graphene depend on the number of layers, the stacking of multi-layers, and rotational orientation. Multiple characterization methods are sensitive to the number of layers including transmission electron microscopy, Low Energy Electron Microscopy, nano-Raman, optical absorption, and scanned probe methods. Another question is the impact of corrugation on electrical properties. Recent AFM measurements prove the impact of the substrate roughness on corrugation. The ultimate reason for the interest in graphene is the high mobility observed by many researchers. The literature shows that mobility depends on the source of the graphene and stacking configuration. A comparison of some of the data will be shown. In addition, the electrical measurements point to interesting nano-scale electrical properties. Quantum confinement and Berry Phase corrections are two examples of quantum phenomena that alter the properties of nano-scale structures. This talk will provide a high level review of the status of graphene metrology.

### 15:45 Invited Speaker

**Using Raman spectroscopy as metrological tool in the study of graphene and other carbon nanostructures**

**Erlon H Ferreira**, *The National Institute of Metrology, Standardization and Industrial Quality, Brazil*

Graphene is a promising material in the development of future nanodevices. Developing methods of characterization and creating metrological standards is an issue of great relevance in this process. Here we present different approaches in the study of defects and deformations in graphene done at the Division of Materials in Inmetro. Raman is the most common technique used to study carbon materials and it is also the most suitable to study the presence of defects in graphene. We have done a thorough analysis of the Raman spectrum of a monolayer graphene as we increase the disorder in the system by a systematic and controlled ion bombardment. In special, the evolution of the intensity ratio between the G band (1585 1/cm) and the disorder-induced D band (1345 1/cm) with ion dose is accurately determined, providing a spectroscopy-based method to quantify the number of defects in that system. This evolution can be fitted by a phenomenological model which is in conceptual agreement with a well-established amorphization trajectory for graphitic materials, but differs substantially from the broadly used Tuinstra-Koening relation for the small disorder. Defects have also been created on HOPG using a focused ion beam (FIB) which delivers high energy ions (30 keV) in a controlled way. Raman spectroscopy is then used for testing FIB performance and shows to be a promising metrological tool to test and compare progresses in ion beam optics for soft modification. Some other applications of Raman spectroscopy in the study of carbon nanostructures will also be addressed.

## ■ *Session: Applications*

### 16:15 Invited Speaker

**Metrology of Single-walled Carbon Nanotube Products Manufactured in Large Scale**

**Daniel Resasco**, *University Of Oklahoma, USA* | **Veronica Irurzun**, *University Of Oklahoma, USA* | **Ricardo Prada**, *SouthWest Nanotechnologies* | **Yongqiang Tan**, *SouthWest Nanotechnologies*

Since June 2008, SWeNT is operating at its 18,000-square-foot manufacturing facility. The new plant has capacity for producing several Kg/day with the CoMoCAT process. The commercial products offered by SWeNT include: SG65 (highly enriched in (6,5) SWCNT type), SG76 (enriched in (7,6) and (8,7) SWNT types), CG200 (broader distribution of chiralities with average diameter of 1.0 nm). CS100 (conductive silica, a nano-hybrid SWNT/SiO2 nanoparticles). Thin SWNT films and nanotube inks, and SMW (special multi-walled carbon nanotubes of narrow diameter). Quality control specifications have been developed, based on established metrology for large-scale batches. The following quality parameters have been established, and the specifications are applied to every sample produced: 1) Raman Parameters (Lambda=D/G, and absolute G intensity). 2) TGA parameters (T1 and R%) 3) Optical Absorption (parameters P2B and S2B) 4) Photoluminescence 5) Suspendability/precipitation factor (P). In this contribution, we describe a method recently implemented to assess the purity of SWCNT bulk samples based on Raman spectroscopy of liquid suspensions. The method has higher reproducibility and quantitative precision than those previously used. It consists of measuring the G-band intensity of liquid suspensions of SWCNT samples as a function of solid concentration. A simple equation is proposed in which one of the two adjustable parameters is the SWCNT purity. The method has been applied to a series of samples of similar characteristics, but varying quality. The results are compared to those obtained on the same series of samples using standard analytical techniques, including electron microscopy, thermogravimetric analysis and optical absorption. "

### 16:45 Invited Speaker

**Structural Characterization of Multi-walled Carbon Nanotubes for Commercial Applications and Safety Issue**

**Morinobu Endo**, *Shinshu University, Japan*

Multi-walled carbon nanotubes (MWNTs) have pursued their end uses in numerous areas (e.g., nanocomposite, energy storage, sensors, field-emission displays, radiation sources, devices, actuator and probes) by exploiting their novel physical and chemical properties derived from their atomistic configurations as well as various geometrical structures. Industrially produced carbon nanotubes reach 1000 ton/year, because the cost-effective catalytic CVD technique for producing carbon nanotubes in a large scale has been established. Therefore, a synergistic effect of an industrially produced carbon nanotubes and the newly created end-uses will cut down their price by at least 10 percent of the current value in the near future. However, there is no standard way to assess the quality of MWNTs, even though their quality is extremely important to make a product with a desired performance. Here I will describe the current status of MWNTs productions, and then their current usages, by suggesting the several important measurement methods to evaluate basic properties of MWNTs and quality of commercial products for standardization as well as safety issue of MWCNTs.

## 17:00 MSIN Poster

### Characterizing Carbon Nanotube Reference Materials

**Jeffrey Fagan**, *National Institute Of Standards And Technology*

NIST has produced and characterized two different carbon nanotube reference materials for upcoming release. These include a certified reference material based on a homogenized batch of raw nanotube soot (SRM 2483) and a set of purified length sorted populations in aqueous dispersion (RM 8281). SRM 2483 will be certified for the elemental composition and homogeneity of the material as evaluated by neutron activation analysis, ICP-MS, an thermogravimetric analysis; informational values with respect to the optical absorbance of the material after dispersion, Raman scattering information, and TEM images will also be detailed. RM 8281, also in use as the round robin candidate for VAMAS TWA 34 project 1 on chirality distribution measurement, will have information including optical properties, and the distribution of lengths within the three fractions. An overview along with details of the characterization process, including development, difficulties encountered along the way, and the projected end use of these materials will be presented.

### Pulsed characterization for hysteresis-free carbon nanotube mobility measurements

**David Estrada**, *University Of Illinois At Urbana-Champaign; Micro and Nanotechnology Laboratory, IL* | **Sumit Dutta**, *University Of Illinois At Urbana-Champaign* | **Albert Liao**, *University Of Illinois At Urbana-Champaign; Micro and Nanotechnology Laboratory, IL* | **Eric Pop**, *University Of Illinois At Urbana-Champaign; Micro and Nanotechnology Laboratory, IL; Beckman Institute for Advanced Science and Technology*

We describe a pulsed voltage measurement method for electrical characterization of carbon nanotube (CNT) transistors. The approach enables consistent, nearly hysteresis-free measurements of CNT mobility and threshold voltage. By contrast, existing DC measurements used for characterization of CNT current vs. gate voltage typically show a strong dependence on the direction of the voltage sweep. This behavior is attributed to charge trapping by surrounding water molecules or charge injection into the nearby substrate. Such hysteresis makes mobility and threshold voltage measurements difficult and unreliable, and is at least in part responsible for the inconsistent CNT mobility data reported thus far in the literature. We have performed pulsed gate voltage measurements over a wide temperature range (80 – 450 K) and found that hysteresis can be reduced by adjusting the pulse off time [1]. This allows trapped charge in the adjacent dielectric (SiO2) to relax, preventing device hysteresis. Comparing pulsed measurements with a tunneling model, we found trap relaxation times of 0.01 – 10 s and trap depths up to 4 – 8 nm. CNT mobility extracted from pulsed measurements is consistent, and comparing it with device simulations reveals the role of transport in multiple sub-bands. By contrast, mobility extracted from DC measurements varies greatly between the forward and reverse gate sweeps. In conclusion, pulsed measurements provide a novel and better approach to extracting the “true” electrical properties of carbon nanotubes. [1] D. Estrada, S. Dutta, A. Liao, E. Pop, Nanotechnology 21, 085702 (2010).

### Indexing of individual SWNTs from Raman spectroscopy

**Thierry Michel**, *LCVN, CNRS-Université Montpellier 2, France* | **Matthieu Paillet**, *LCVN, CNRS-Université Montpellier 2, France* | **Denise Nakabayashi**, *LCVN, CNRS-Université Montpellier 2, France* | **Mathieu Picher**, *LCVN, CNRS-Université Montpellier 2, France* | **Vincent Jourdain**, *LCVN, CNRS-Université Montpellier 2, France* | **Jannick Meyer**, *University of Ulm, Ulm, Germany* | **Amhed Zahab**, *LCVN, CNRS-Université Montpellier 2, France* | **Raul Arenal**, *LEM, ONERA, France* | **Romain Fleurier**, *LEM, ONERA, France* | **Jean-Louis Sauvajol**, *LCVN, CNRS-Université Montpellier 2, France*

From combined Raman spectroscopy and electron diffraction studies on several freestanding single-walled carbon nanotubes (SWNT), we define Raman criteria which correlate the main features of the Raman spectrum (Radial Breathing Mode and G-modes) with the structure of the SWNT under investigation. On this basis, we discuss the possibilities to determine the (n,m) indices of an individual SWNT from a single wavelength Raman experiment. We show the efficiency of this approach in assigning the (n,m) structure of different individual nanotubes including all types of achiral SWNTs. Finally, the limits and the accuracy of the method are discussed.

### Optical Absorption Spectroscopy of Single-Wall Carbon Nanotubes, A Standard Method for Characterizing the Diameter

**Takeshi Saito**, *National Institute of Advanced Industrial Science and Technology (AIST)* | **Shigekazu Ohmori**, *National Institute of Advanced Industrial Science and Technology (AIST)* | **Bikau Shukla**, *National Institute of Advanced Industrial Science and Technology (AIST)* | **Motoo Yumura**, *National Institute of Advanced Industrial Science and Technology (AIST)* | **Sumio Iijima**, *National Institute of Advanced Industrial Science and Technology (AIST)*

An unique potentiality of optical absorption spectroscopy (OAS) for the estimation of mean diameter of single-wall carbon nanotubes (SWCNTs) from observed electronic transition energies has been explored. It is worth noting that this investigation has contributed to standardization activity of ISO TC229, that is, Technical Specification for the characterization of SWCNTs using OAS (ISO/DTS10868). The observed interdependency of electronic transition energies of both metallic and semiconducting SWCNTs on their mean diameters clearly showed that transition energies inversely scale with the diameters. The detailed analysis of the results allowed us to formulate the correlation between them as follows: Eg(S11)=0.96/dm, Eg(S22)=1.7/dm, and Eg(M11)=2.6/dm, where Eg is the transition energy and dm is the mean diameter. Resulted formulas have been found applicable for determinning mean diameter of SWCNTs directly from their observed optical absorption peaks in the wide range of diameters, ca. 1-2 nm. Thus, output of this result is expected to be useful for characterizing the mean diameter of SWCNTs, as a complement/ alternative method to the similar analysis done by resonance Raman spectroscopy. This work has been partially supported by New Energy and Industrial Technology Development Organization (NEDO) project.

### CNTs.org: A New Centralized, Open-Source Platform for Standardizing, Sharing Methods, and Reaching Consensus on Mechanisms Related to Nanostructured Carbon Materials

**Stephen Steiner III**, *Massachusetts Institute of Technology*

Open-source methodology has been tremendously successful in mobilizing large bodies of people to collaboratively develop and deploy advanced software technologies. We propose applying the same approach to the lab-scale production, medium-scale manufacture, characterization, and application of nanostructured carbon materials. CNTs.org is a new project aimed at providing a free, centralized collaborative platform for sharing how-to guides for building CVD systems and growing CNTs, graphene, and diamond materials; democratically reaching consensus on important mechanistic details; publicly sharing and standardizing characterization methods; providing basic reference and instructional guides; and quickly disseminating results and observations. This poster summarizes the goals and proposed timeline of the project and invites participants of NT10 to volunteer to help seed the initial content of the effort.

## Quantitative Determination of the Metallic/Semiconducting Ratio of Bulk Single-Walled Carbon Nanotube Samples by Cobalt Porphyrin Probe EPR Spectroscopy

**Sofie Cambré**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Wim Wenseleers**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Etienne Goovaerts**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Daniel E. Resasco**, *School of Chemical, Biological and Materials Engineering, University of Oklahoma,*

In recent years, significant progress was made in the preparation of SWCNT samples enriched in either semiconducting (SC) or metallic (M) tubes, either at the synthesis level or by various post growth separation methods. However, characterizing the actual content of semiconducting and metallic SWCNTs in a bulk sample remained difficult, because no simple spectroscopic assay giving a reliable, absolute reading of the M:SC ratio for SWCNT samples of arbitrary diameter distribution was available till now. Here, we show that the EPR spectrum of a bulk sample of SWCNTs, to which Co(II)octaethylporphyrin (CoOEP) probe molecules have been added, directly yields such a measurement of the M:SC ratio (mass%) in the original SWCNT sample, without requiring an external calibration, yielding a simple, quantitative spectroscopic technique for the determination of M:SC ratios in bulk SWCNT samples.[1] This assay is based on our previous finding that the significantly different interaction of metallic and semiconducting SWCNTs with CoOEP is readily resolved in EPR spectra,[2] and on the intrinsically quantitative nature of EPR. Experiments show that the EPR spectra are independent of other aspects such as diameter or synthesis method. [1] S. Cambré, W. Wenseleers, E. Goovaerts, D.E. Resasco, 'Determination of the Metallic/Semiconducting Ratio in Bulk Single-Walled Carbon Nanotube Samples by Cobalt Porphyrin Probe EPR Spectroscopy' (to be published). [2] S. Cambré, W. Wenseleers, J. Culin, S. Van Doorslaer, A. Fonseca, J. B.Nagy & E. Goovaerts, 'Characterisation of nanohybrids of porphyrins with metallic and semiconducting carbon nanotubes by EPR and optical spectroscopy' ChemPhysChem 9, 1930-1941 (2008).

## The Kataura plot

**Ado Jorio**, *UFMG* | **Paulo Araujo**, *UFMG* | **Jaqueline Soares**, *UFMG* | **Luiz Gustavo Cancado**, *UFMG* | **Cristiano Fantini**, *UFMG* | **Mildred Dresselhaus**, *MIT* | **Kentaro Sato**, *Tohoku University* | **ART Nugraha**, *Tohoku University* | **Riichiro Saito**, *Tohoku University*

Here the latest developments for assigning the (n,m) indices to the radial breathing mode frequencies and optical transition energies of single wall carbon nanotubes are discussed. The environmental effects are addressed trying to make a generalization on how to build the Kataura plot for different samples which have already been established, plus the constrains one should consider when is dealing with a new samples that has never been measured.

# 3rd Carbon Nanotube Biology, Medicine and Toxicology Satellite Symposium (CNBMT10)

**Organizers:**
**Alberto Bianco**,*Institut de Biologie Moléculaire et Cellulaire, CNRS, France*
**Emmanuel Flahaut**, *Université Paul Sabatier, CNRS, France*
**Marianna Foldvari**,*School of Pharmacy,University of Waterloo, Canada*
**Kostas Kostarelos,** *The School of Pharmacy, University of London, UK*
**Masako Yudasaka**, *National Institute of Advanced Industrial Science and Technology [AIST], Japan*

## ROOM: WESTMOUNT

## Sunday, June 27

### 8:50-9:00 OPENING

**1st Section CELL BIOLOGY**

### 9:00-9:35 Invited Speaker

**A New Platform for Studying Cell Signaling: Near Infrared Fluorescent Carbon Nanotube Arrays with Single Molecule Sensitivity**
**Michael Strano**, *MIT, USA*

The 1D quantum confinement of photogenerated excitons in single-walled carbon nanotubes (SWNT) can amplify the fluorescent detection of molecular adsorption to where single-molecule discrimination is realizable, even from within living cells and tissues. This attribute sets the carbon nanotube apart from virtually all biosensor platforms in existence. Our laboratory has been applying these new types of sensors and sensor arrays to solve difficult or unaddressed problems in biochemical signaling in cellular systems. After reviewing the synthesis, properties and mathematical analysis of such sensors as applied to biological signaling, several case studies will be examined. Nitric oxide (NO) releasing drugs are promising anti-cancer agents but the study of their activity in cellular systems is complicated by the difficulty in measuring NO relative to its decomposition products. We have designed amphiphilic polymers that wrap the nanotube and impart selectivity and single molecule sensitivity to NO, enabling detection, even in-vivo. Current efforts focus on the study of NO release kinetics and methods to improve the stability and delivery of NO releasing drugs. We have also solved an important problem in epidermal growth factor receptor signaling. An emerging concept in cell signalling is the natural role of reactive oxygen species such as hydrogen peroxide (H2O2) as beneficial messengers in redox signalling pathways. In spite of the growing evidence, the nature of H2O2 signalling is confounded by difficulties in tracking it in living systems, both spatially and temporally, at low concentrations. I will discuss our efforts to develop an array of fluorescent single-walled carbon nanotubes that can selectively record, in real time, the discrete, stochastic quenching events that occur as H2O2 molecules are emitted from individual human epidermal carcinoma cells stimulated by epidermal growth factor. We show mathematically that such arrays can distinguish between molecules originating locally on the cell membrane from other contributions. We also use this analytical tool to elucidate the biochemical pathway of this signaling for the first time. I will finish by commenting on extensions of this platform to angiogenic signaling and dopamine signaling in neurological systems.

### 9:35-9:50 Contributed Talk

**Double-walled carbon nanotubes for neural tract engineering**
**Amelie Beduer**, *CNRS, LAAS, France* | **Florent Seichepine**, *CNRS, LAAS, France; Université de Toulouse ; UPS, INP ; Institut Carnot Cirimat ; France* | **Laurence Vaysse**, *INSERM ; Imagerie Cerebrale et Handicaps Neurologiques UMR 825 ; France.* | **Isabelle Loubinoux**, *INSERM ; Imagerie Cerebrale et Handicaps Neurologiques UMR 825 ; France.* | **Christophe Vieu**, *CNRS, LAAS, France* | **Emmanuel Flahaut**, *Université de Toulouse ; UPS, INP ; Institut Carnot Cirimat ; France; CNRS; Institut Carnot Cirimat; France*

Carbon nanotubes (CNT) are currently investigated for many biomedical applications, ranging from medical imaging (MRI) to targeted drug delivery and biological sensing. Tissue engineering is a field in which CNT could bring many improvements as compared to existing biomaterials, and especially for regeneration of neuronal tissues as they provide a unique combination of useful electrical and mechanical properties at the nanometer scale. Our results show that through surface engineering, we can direct and guide the growth and differentiation of neural cells. Topographical grooves obtained by a moulding process against a silicon master turned efficient for both neural lines cells and adult neural stem cells. Double-walled CNT [1] patterns obtained by soft lithography were also found very efficient and have the advantage of possible electrical stimulation due to their metallic electrical behaviour.
In both cases, low cost fabrication processes (moulding or soft&#8208;lithography) are developed, enabling further large scale applications for biological or medical purposes. References: [1] E. Flahaut et al., Chem. Comm. (2003) 1442

### 9:50-10:05 Contributed Talk

**Open slot**

### 10.05-10.25 COFFEE BREAK

**(POSTER SESSION)**

### 10:25-10:40 Contributed Talk

**Open slot**

## ■ *2nd Section IMAGING*

### 10:40-11:15 Invited Speaker

**Imaging the Cellular Uptake of Multi-walled Carbon Nanotubes using 3-D Electron Tomography**
**Alexandra Porter**, *Imperial College London, United Kingdom*
**Khuloud Al-Jamal**, *Nanomedicine Lab, School of Pharmacy, Centre for Drug Delivery Research, University of London, UK* | **Hannah Nerl**, *Imperial College London, United Kingdom* | **Jeorg Jinshck**, *The FEI Company, Eindhoven, Holland.* | **Karin Muller**, *Imperial College London, United Kingdom* | **Hanne Ali-Boucetta**, *Nanomedicine Lab, School of Pharmacy, Centre for Drug Delivery Research, University of London, UK* | **Alberto Bianco**, *CNRS Institut de Biologie Moléculaire et Cellulaire, France* | **Maurizio Prato**, *Center of Excellence for Nanostructured Materials, University of Trieste, Italy* | **Kostas Kostarelos**, *Nanomedicine Lab, School of Pharmacy, Centre for Drug Delivery Research, University of London, UK*

Functionalised and surface coated carbon nanotubes (CNTs) are being investigated for use as carriers for targeted drug delivery and diagnostic agents. Despite extensive study, little is known about the effect of surface modification on the pathway by which CNTs enter cells or their long term fate. The “nanoneedle” hypothesis [1], of direct penetration into cells by CNTs, has been a controversial proposition and its visualization has been achieved in 2D only. We exposed A549 epithelial and human macrophage cells (HMMs) to two fundamentally different types of shortened multi-walled carbon nanotubes (MWNTs): NH3+-functionalised MWNTs (MWNT-NH3+), and non-functionalised co-polymer (Pluronic F127) coated (p-MWNTs). Using a combination of 3-D electron tomography and energy filtered transmission electron microscopy, we confirmed that uptake of chemically ammonium functionalised MWNT by epithelial cells was significantly greater than the p-MWNTs. Both the MWNT-NH3+ and the p-MWNTs inserted into the plasma membrane of cells via direct penetration, whereas the MWNT- NH3+ were also found engulfed by endosomal-dependent pathways in addition to direct penetration. There was no difference in degree of uptake between the two MWNTs types in HMMs. Incubation of cells with MWNTs at 4 &#61616;C greatly reduced, but not completely inhibited the uptake of MWNTs in both cell types, especially HMMs. After 14 days, the MWNT- $NH_3^+$ had escaped the lysosomes and distributed over the cytoplasm. This study confirms that both cell type and nature of surface functionalization determine the extent and mechanism of cellular uptake.  [1] Pantarotto D. Angew Chem Int Engl. 4 (2004) 43(39):5242-6.

## 11:15-11:30  Contributed Talk

### Synthesis of 14C-labelled Carbon Nanotubes for in vivo biodistribution studies

**Mathieu Pinault**, *CEA Saclay - Laboratoire Francis Perrin CEA CNRS URA 2453, France* | **S Habib**, *CEA Saclay - Laboratoire Francis Perrin CEA CNRS URA 2453, France* | **D Georgin**, *CEA, IBITECS, Service de Chimie Bioorganique et de Marquage* | **F Taran**, *CEA, IBITECS, Service de Chimie Bioorganique et de Marquage* | **B Czarny**, *CEA, IBITECS, Service d'Ingénieurie Moléculaire des Protéines* | **B Bouchet Fabre**, *CEA Saclay - Laboratoire Francis Perrin CEA CNRS URA 2453, France* | **M Carrière**, *CEA IRAMIS SIS2M* | **JL Poncy**, *CEA, IRCM, Laboratoire de Radiotoxicologie* | **R Maximilien**, *CEA, IRCM, Laboratoire de Radiotoxicologie* | **V Dive**, *CEA, IBITECS, Service d'Ingénieurie Moléculaire des Protéines* | **M Mayne L'hermite**, *CEA Saclay - Laboratoire Francis Perrin CEA CNRS URA 2453, France*

Carbon nanotubes (CNT) are currently developed for multiple future commercial applications. It is therefore more than ever necessary to address their health safety implications and in particular explore their in vivo biodistribution and pharmacokinetics. One critical point for such investigation is the labelling strategy of CNT in order to track their behavior and fate in the body that could lead to some surface modifications influencing interactions of CNT with biological materials. In a first step we developed a new post treatment method that allows the 14C-labeling of purified MWCNT without modifying their structure. Results of a preliminary biodistribution study in rats will be presented3. However, MWCNT produced through this method could not reach a sufficient 14C-labeling level for in vivo bio-persistence studies. In order to increase the specific activity of the 14C-labelled MWCNT we developed a process based on the previously reported aerosol-assisted CCVD process4. For the first time, MWCNT were synthesized by the direct use of 14C-labelled benzene as the carbon source and were fully characterized (SEM, TEM, TGA). Long and aligned CNT (controllable length around 100μm, mean external diameter of 40 nm) that are uniformly radiolabelled with a very high specific activity (more than 100 μCi/mg) have been formed. Thanks to the high specific activity of these 14CNT, low quantity (~1μg) of CNT will be used to contaminate a series of rats. Further in vivo experiments will be designed to evaluate the eventual bio-accumulation and bio-persistence of CNT.

## 11:30-11:45 Contributed Talk

### Gd@DWNT: A new high relaxivity contrast agent for MRI

**Carmen - Mihaela Tîlmaciu**, *Université de Toulouse, France* | **Brigitte Soula**, *Université de Toulouse, France* | **Anne-Marie Galibert**, *Université de Toulouse, France* | **Florian Gimbert**, *UFR de Sciences Pharmaceutiques, France* | **Thibaut Dubois**, *UFR de Sciences Pharmaceutiques, France* | **Petar Lukanov**, *Université de Toulouse, France* | **Isabelle Loubinoux**, *INSERM UMRS 825, Service de Neurologie, , France* | **Soraya Benderbous**, *UFR de Sciences Pharmaceutiques, France; INSERM UMRS 825, France* | **Emmanuel Flahaut**, *CNRS, Institut Carnot Cirimat, France*

MRI contrast agents are widely used in clinical routine, because of their ability to decrease the relaxation times of protons from the surrounding water. Recent studies highlight Gadonanotubes (Gd@CNT) [1] as a new challenging material, which is expected to have a higher efficiency than the current contrast agents with low relaxivity (e.g. gadolinium complex). In this work, narrow double-walled carbon nanotubes (DWNT) synthesized by CCVD [2] and purified in air [3] were filled with $GdCl_3$ in melted phase. Several washing procedures were tested to improve the purity of the Gd@DWNT. HRTEM, EDX and elemental analysis were performed, in order to evidence the filling and to quantify the yield of Gd(III) in the samples. A major objective of the research is to make neuronal imaging using these Gd@DWNT. Preliminary measurements of relaxation times and control if possible leaks were achieved on several samples with different concentrations of gadolinium. The results are encouraging: a good stability in time (over six months) and high relaxivities of the Gd@DWNT (about five times greater than the current main clinical agent).   References: [1] B. Sitharaman et al., Int. J. Nanomed., (2006), 291 [2] E. Flahaut et al., Chem. Commun., (2003), 1442 [3] S. Osswald et al., Chem. Mater., 18, (2006), 1525

## 11:45-12:00  Contributed Talk

### Detection of single-molecule $H_2O_2$ signalling from epidermal growth factor receptor using fluorescent single-walled carbon nanotubes

**Hong Jin**, *Massachusetts Institute of Technology, USA* | **Jingqing Zhang**, *Massachusetts Institute of Technology, USA* | **Hyeonseok Yoon**, *Massachusetts Institute of Technology, USA* | **Michael Strano**, *Massachusetts Institute of Technology, USA*

An emerging concept in cell signalling is the natural role of reactive oxygen species such as hydrogen peroxide ($H_2O_2$) as beneficial messengers in redox signalling pathways. In spite of the growing evidence, the nature of $H_2O_2$ signalling is confounded by difficulties in tracking it in living systems, both spatially and temporally, at low concentrations. Here, we develop an array of fluorescent single-walled carbon nanotubes that can selectively record, in real time, the discrete, stochastic quenching events that occur as $H_2O_2$ molecules are emitted from individual human epidermal carcinoma cells stimulated by epidermal growth factor.(Jin, et al. 2008; Jin, et al. 2010) We show mathematically that such arrays can distinguish between molecules originating locally on the cell membrane from other contributions. We find that epidermal growth factor induces 2 nmol $H_2O_2$ locally over a period of 50 min. This platform promises a new approach to understanding the signalling of reactive oxygen species at the cellular level.  Jin, H., et al. (2010). 'Detection of single-molecule $H_2O_2$ signalling from epidermal growth factor receptor using fluorescent single-walled carbon nanotubes.' Nature Nanotechnology (Submitted).  Jin, H., et al. (2008). 'Stochastic analysis of stepwise fluorescence quenching reactions on single-walled carbon nanotubes: single molecule sensors.' Nano letters 8(12): 4299-4304.

## 12:00 LUNCH

**(POSTER SESSION)**

## ■ *3rd Section THERAPY*

## 14.00-14.35 Invited talk

### In vivo gene delivery by tetra (piperazino) fullerene epoxide (TPFE)

**Eisei Noiri**, *The University of Tokyo Hospital, Japan* | **Hiroyuki Isobe**, *Chemistry, Tohoku University* | **Rui Mamiya-Maeda**, *The University of Tokyo Hospital, Japan* | **Waka Nakanishi**, *Chemistry, Tohoku University* | **Tatsuya Homma**, *Chemistry, The University of Tokyo* | **Koji Okamoto**, *The University of Tokyo Hospital, Japan* | **Kent Doi**, *The University of Tokyo Hospital, Japan* | **Eiichi Nakamura**, *Chemistry, The University of Tokyo*

Water-soluble fullerenes are molecules with great potential for biological use because they can endow unique characteristics of amphipathic property and form a self-assembled structure by chemical modification. Based on the previous report of effective gene delivery in vitro with tetra (piperazino) fullerene epoxide (TPFE) and its superiority to Lipofectin, we evaluated the efficacy of in vivo gene delivery by TPFE in this study. Delivery of enhanced green fluorescent protein gene (EGFP) by TPFE on pregnant female ICR mice showed distinct organ selectivity compared with Lipofectin; moreover, higher gene expression by TPFE was found in liver and spleen, but not in the lung. No acute toxicity of TPFE was found for the liver and kidney, although Lipofectin significantly increased liver enzymes and blood urea nitrogen. In fetal tissues, neither TPFE nor Lipofectin induced EGFP gene expression. Delivery of insulin 2 gene to female C57/BL6 mice increased plasma insulin levels and reduced blood glucose concentrations, indicating the potential of TPFE-based gene delivery for clinical application. In conclusion, this study demonstrated effective gene delivery in vivo for the first time using a novel water-soluble fullerene.

### 14:35-14:50 Contributed Talk

**Open slot**

### 14:50-15:05 Contributed Talk

**Open slot**

### 15:05-15:25 COFFEE BREAK

**(POSTER SESSION)**

## ■ 4th Section TOXICOLOGY

### 15:25-16:00 Invited talk

**Establishing carbon nanotube biocompatibility parameters for their application as pharmaceutical excipients for nanomedicines**

**Marianna Foldvari**, *University of Waterloo, Canada*

Many of the recently designed drug delivery systems are constructed from nano-sized components that serve as the carrier or targeting ligand for a therapeutic agent. Even though these biomaterials have been regarded in the past as inert or non-active components of dosage forms, they are now recognized as being sometimes even more important than the drug itself. Hence, it is becoming increasingly important that the pharmaceutically relevant properties, including toxicity, of these functional nano-excipients be fully characterized. One group of biomaterials, carbon nanotubes (CNTs), have potential as pharmaceutical excipients due to their versatile structural properties such as high aspect ratio, propensity for surface functional modification, internal cavity for drug encapsulation and transfer and potential biocompatibility that are particularly useful for pharmaceutical nanodelivery. The desirable and undesirable ‘nano-effects’ of carbon nanotubes and their composites, used as pharmaceutical excipients, on cellular function will be discussed. Initiatives for the construction of a physicochemical database for functional nano-excipients that will assist in establishing correlation between their physical, chemical, morphological and intelligent properties and their biological effects in vivo, will be described.

### 16:00-16:15 Contributed Talk

**Sharper and Faster Nano Darts Kill More Bacteria: A Study of Antibacterial Activity of Individually Dispersed Pristine Single-Walled Carbon Nanotube**

**Yuan Chen**, *Nanyang Technological University, Singapore* | **Shaobin Liu**, *Nanyang Technological University, Singapore* | **Li Wei**, *Nanyang Technological University, Singapore*

To further our understanding on the antibacterial activity of single-walled carbon nanotubes (SWCNTs), high purity SWCNTs with average diameter of 0.83 nm and (7,5) chirality as dominate (n,m) structure were dispersed in a biocompatible surfactant solution. Ultraviolet visible near-infrared radiation absorption spectroscopy was employed to monitor the aggregation of SWCNTs. The results demonstrated that individually dispersed SWCNTs were more toxic than SWCNT aggregates toward bacteria (gram-negative Escherichia coli, Pseudomonas aeruginosa, and gram-positive Staphylococcus aureus, Bacillus subtilis). Individually dispersed SWCNTs can be visualized as numerous moving ¡°nano darts¡± in the solution, constantly attacking the bacteria; thereby, degrading the bacterial cell integrity and causing the cell death. Controlled experimental results suggested that inhibiting cell growth and oxidative stress were not the major causes responsible for the observed death of cells. Furthermore, the detrimental effects of Co metal residues (up to 1 ug/mL) on SWCNT samples can be ruled out. Atomic force microscope study conducted in suspension proved that the death rates of bacteria were strongly correlated with their mechanical properties; soft cells were more vulnerable to SWCNT piercing. This study elucidated several factors controlling the antibacterial activity of pristine SWCNTs and it provided an insight in developing strategies that can maximize the SWCNT application potentials while minimizing the health and environment risks.

### 16:15-16:30 Contributed Talk

**Toxicology Study of Single-Wall Carbon Nanohorns with Different Sizes Intravenously Administrated in Mice**

**Minfang Zhang**, *National Institute Of Advanced Industrial Science And Technology, Japan* | **Takashi Yamaguchi**, *Nagoya University* | **Sumio Iijima**, *National Institute Of Advanced Industrial Science And Technology, Japan; Nagoya University; NEC; Meijo University* | **Masako Yudasaka**, *National Institute Of Advanced Industrial Science And Technology, Japan; NEC*

With the study of carbon nanotubes on biomedical applications, their toxicity is a critical issue. It has been realized that the toxicity of nanotubes is related to their length and impurities. However, the knowledge on toxicity of carbon nanotubes is still limited. Herein, we have studied the immune toxicities and biodistribution of single-wall carbon nanohorns (SWNHs) which were intravenously administered in mice. We used SWNHs with two different aggregate-sizes: 80-120 nm and 30-50 nm. The latter ones were separated from the former ones by sucrose gradient centrifuge. The hematologic test showed that the blood counts and the differential counts of white blood cells did not show much difference between two types of SWNHs and control PBS. The measurements of proinflammatory cytokines revealed that there were no significant releases of TNF-ƒ¿, IFN-ƒÁ and IL-6 whatever samples were injected. The biodistribution of SWNHs were investigated by using Gd2O3 labeled SWNHs. The results showed that the blood circulation time of SWNHs with small sizes were longer (about 6 h) than that of SWNHs with larger sizes (<1 h). After 24 h since the administration, both of two sized SWNHs were mainly localized in liver and spleen, and significantly, a few of SWNHs (about 5%) existed in intestines. We also found trace amount of SWNHs in feces from one mouse, suggesting that SWNHs could be excreted from mouse.

### 16:30-16:45 Contributed Talk

**Open slot**

## ■ 5th Section ENVIRONMENTAL IMPACT

### 16:45-17:20 Invited talk

**Enzymatic biodegradation of carbon nanotubes: Environmental and health implications**

**Alexander Star**, *University of Pittsburgh, USA*

Because of their unique properties, such as high tensile strength, chemical stability, and electrical conductivity, carbon nanotubes are an ideal material for many commercial applications. As nanotube applications progress in number and variety, so do the altering environments in which they are implemented. Yet, no consensus regarding the environmental and human toxicity factors of these materials exists. We have recently investigated the enzymatic degradation of single-walled carbon nanotubes (SWNTs). Use of peroxidase enzymes such as horseradish peroxidase (a common plant enzyme) and human myeloperoxidase (secreted by physiological neutrophils) have shown oxidative capabilities to degrade carboxylated SWNTs. Low localized concentrations of H2O2 (~40 μM), in combination with these peroxidases, initiate the degradation of SWNTs in approximately 10 days at room temperature and 24 hours at body temperature. Moreover, it has been demonstrated that completely degraded products (consisting primarily of CO2) elicit no toxicological response. Mechanistic investigations have attributed enzymatic degradation to surface oxygen functionalities of SWNTs interacting with positively charged amino acid residues of both enzymes, leading to close proximal contact with the active oxidizing heme sites contained therein. Our results indicate that SWNTs might have limited persistence of in the environment and that there are may be physiological mechanisms exist for their biodegradation.

## 17:20-17:35 Contributed Talk

### Comparative ecotoxicological study in water of double and multi walled carbon nanotubes

**Périne Landois**, *CEA-Saclay Laboratoire Francis Perrin, France; Institut Carnot Cirimat, France* | **Florence Mouchet**, *EcoLab (Laboratoire d'écologie fonctionnelle) , France* | **Pascal Puech**, *CEMES, France* | **Laury Gauthier**, *EcoLab (Laboratoire d'écologie fonctionnelle), France* | **Emmanuel Flahaut**, *Institut Carnot Cirimat, France*

The increased production of carbon nanotubes (CNT) raises questions about their potential effect on health and environment and therefore justifies the need for studies in this direction. A comparative study of the effect of CNT on amphibian larvae in aquatic media (ultimate receptacle of all pollution) will be presented. The potential impact of carbon nanotubes was investigated under normalised laboratory conditions according to the International Standard micronucleus assay (ISO 21427-1) for 12 days of half-static exposure in water. Three different endpoints were carried out for 12 days of exposure: mortality, growth inhibition, and micronuclei induction in erythrocytes in the circulating blood of larvae. Raman spectroscopy analysis was used to investigate the presence of CNT in the biological samples. Considering the high diversity of CNT according to their different characteristics, multi-walled carbon nanotubes were analyzed in Xenopus larvae, comparatively to double-walled carbon nanotubes in similar conditions. Growth inhibition in larvae exposed to CNT was also evidenced, and no genetoxicity (micronucleus assay) was noticed, whatever the concentration as in the case of DWNT. CNT localisation in the larvae leads to different possible hypothesis of mechanisms explaining toxicity in Xenopus. These results will be presented and discussed insisting on the difficulties of current assays of ecotoxicity of carbon nanotubes.

## 17:35-17:50 Contributed Talk

### Open slot

## 17:50-18:00 CLOSING REMARKS

## LIST OF POSTER PRESENTATIONS

### Influence of cell-penetrating carbon nanotubes on siRNA transfection in primary astrocyte cultures

**Camila Marques Freria**, *Laboratory of Nervous Regeneration, Institute of Biology, University of Campinas, Brazil.* | **Diego Stéfani**, *LQES-Solid State Chemistry Laboratory, Institute of Chemistry, University of Campinas, Brazil.* | **Renata Grazieli Zanon**, *Laboratory of Nervous Regeneration, Institute of Biology, University of Campinas, Brazil.* | **Antônio Gomes Souza Filho** ,*LQES-Solid State Chemistry Laboratory, Institute of Chemistry, University of Campinas, Brazil.; Department of Physics, Federal University of Ceará, Brazil.* | **Josué Mendes Filho**, *Department of Physics, Federal University of Ceará, Brazil.* | **Alexandre L. R. Oliveira**, *Laboratory of Nervous Regeneration, Institute of Biology, University of Campinas, Brazil.* | **Oswaldo Luiz Alves**, *LQES-Solid State Chemistry Laboratory, Institute of Chemistry, University of Campinas, Brazil.*

The applications of carbon nanotubes (CNTs) in biological systems are attracting considerable attention of the scientific community. In particular, the interactions of CNTs with nervous system cells have become an intriguing and challenging subject which may contribute to the development of new disease treatment and repair approaches. In the present work, the interaction of multi-walled carbon nanotubes (MWCNTs) with rat primary astrocytes cells was investigated by evaluating the glial fibrillary acidic protein (GFAP) expression as well as the MWCNTs ability to transfect small interference RNA (siRNA). The MWCNTs samples used in this work were purified using nitric acid, sodium hydroxide and chloridric acid aiming at obtaining a sample with reduced amount of amorphous carbon and remaining catalysts particles. The MWCNTs samples were characterized by several techniques (TEM-Transmission Electron Microscopy, EDS-SEM, BET, Zeta potential, Thermogravimetric analysis and Raman spectroscopy) allowing to access the structural, morphological, chemical, and surface properties which are relevant for understanding the CNTs-Cell interactions. The results showed that the used MWCNT samples present low citotoxicity and induced an increase of GFAP levels in astrocyte cultures 3 days after exposure. Intracellular fluorescence (siRNA-CY3) was used for monitoring the siRNA transfection into astrocytes using CNTs as transporter. Cell-penetrating carbon nanotubes were confirmed by TEM that revealed both isolated and small bundles of MWCNT inside the cytoplasm of cultured cells. The present findings indicate the possibility of developing new strategies for studying molecular biology processes using cultured glial cells.

### Carbon nanotubes enhanced antibody response in genetically selected mice

**Diego Stéfani**, *LQES-Solid State Chemistry Laboratoy, Institute of Chemistry, University of Campinas, Brazil.* | **Luciana V. Carvalho**, *Laboratory of Immunochemistry, Butantan Institute, Brazil.* | **Antônio G. Souza Filho**, *LQES-Solid State Chemistry Laboratoy, Institute of Chemistry, University of Campinas, Brazil.; Departament of Physics, Federal University of Ceará, Brazil.* | **Osvaldo A. Sant'Anna**, *Laboratory of Immunochemistry, Butantan Institute, Brazil.* | **Oswaldo L. Alves**, *LQES-Solid State Chemistry Laboratoy, Institute of Chemistry, University of Campinas, Brazil.*

In this work we evaluated the immunomodulatory effect of the Multiwall carbon nanotubes (MWNTs) in genetically selected mice for high [HIII] and low [LIII] immunoresponsiveness. Purified MWNTs were characterized by different physico-chemical techniques aiming to access their structural, morphological and surface properties. In vitro experiments have showed that BSA adsorbs in our purified MWNTs. Mice groups were immunized by the subcutaneous route with BSA, BSA in Aluminum hydroxide, BSA adsorbed MWNTs and BSA and MWNTs separately. Blood was collected at different period after immunizations and ELISA was used for IgG titration. The MWNTs enhanced antibody response and induced an efficient immunological memory in both HIII and LIII mice similar to Aluminum hydroxide. The adsorption behavior of BSA on MWNTs surface plays a crucial role for this immunostimulant effect. Finally, we are have shown that carbon nanotubes exhibit a real potential for vaccine delivery through the enhancement of antigen immunogenecity in populations with distinct immunogenetic backgrounds.

### Toxicity and Biodistribution of Hole-Opened Carbon Nanohorns

**Jin Miyawaki**, *Japan Science and Technology Agency, Japan* | **Minfang Zhang**, *Japan Science and Technology Agency, Japan; Advanced Industrial Science and Technology, Japan* | **Sumio Iijima**, *Japan Science and Technology Agency, Japan; Advanced Industrial Science and Technology, Japan; Meijo University, Japan* | **Masako Yudasaka**, *Japan Science and Technology Agency, Japan; Advanced Industrial Science and Technology, Japan*

For drug delivery applications of single-walled carbon nanohorns (SWNHs), toxicity and biodistribution of SWNHs should be clarified. In this report, we show the biodistribution of hole-opened SWNHs (oxSWNHs) and their functionalized species, which was clarified by careful histological observations. The oxSWNH specimens were intravenously injected into mice from tail veins (dosage: 6 mg/kg). No lesions and no abnormality were found, indicating low toxicity of oxSWNHs, which coincided with previous results [1]. Highly hydrophobic oxSWNHs formed large agglomerates, even running up to 50 micrometers, and got stuck in lung vessel lumens. The large agglomerates refused the uptake by macrophages. Interestingly they were partly cleared from lungs: We inferred that this removed portion could be excreted through trachea, because the increase of oxSWNH amount was not found in other organs. The accumulation of oxSWNHs in lungs remarkably reduced, while those in livers, spleens and other organs increased by the functionalization of oxSWNHs with hydrophilic groups. The agglomerate sizes indeed decreased by the hydrophilic functionalization. However, this tendency failed when the attached moiety was BSA. BSA-attached SWNHoxs were highly hydrophilic, but gathered to form large agglomerates in the lung interstitium and their number and size increased with time. The influences of chemical functionalization of oxSWNHs on the biodistribution are largely understood by considering interactions of oxSWNHs with macrophages. Reference: [1] J. Miyawaki, et al., ACS Nano, 2, 213-226 (2008).

### Toxicity and imaging of chemically modified multi-walled carbon nanotubes inhuman macrophage cells

**Slawomir Boncel**, *Department of Organic Chemistry, Biochemistry and Biotechnology, Silesian University of Technology, Poland* | **Karin Müller**, *Multi-Imaging Centre, Department of Physiology, Development and Neuroscience, Anatomy School, University of Cambridge, United Kingdom* | **Jeremy Skepper**, *Multi-Imaging Centre, Department of Physiology, Development and Neuroscience, Anatomy School, University of Cambridge, United Kingdom* | **Andrzej Gondela**, *Department of Organic Chemistry, Biochemistry and Biotechnology, Silesian University of Technology, Poland* | **Krzysztof Walczak**, *Department of Organic Chemistry, Biochemistry and Biotechnology, Silesian University of Technology, Poland* |**Krzysztof Koziol**, *Department of Materials Science and Metallurgy, University of Cambridge, The United Kingdom*

Viability assays revealed a dose dependent toxicity for unpurified and purified (iron-free) multi-walled carbon nanotubes (MWNTs) while imaging provided clues to their active and passive cell penetration into the cytoplasm and nucleus [1]. It was suggested that MWNTs enter cells actively and passively via incomplete phagocytosis or impalation what may result in oxidative stress and cell death from compromised membrane integrity. On the other hand, chemically modified MWNTs are considered as potential drug delivery systems (e.g. in covalent conjugates with biologically active molecules) for cancer therapy due to their capability of both nano-needle behaviour and enhanced excretion [1]. In order to evaluate the toxicity of chemically modified MWNTs we exposed mature human monocyte-derived macrophages (HMM) to oxidised O-MWNTs (6% wt. oxygen in form of highly polar carboxylic –COOH and phenolic groups –OH) and nitrogen doped N-MWNTs (of high crystalline order and nitrogen content 3% wt.). Initial toxicity studies based on the Neutral Red assay revealed no significant decrease in cell viability when incubated with pristine MWNTs, modified O-MWNTs and N-MWNTs, even at such high doses as 20 μg/mL. Furthermore, comparative quantitative toxicological analysis was obtained by a Live/Dead assay using confocal microscopy. In order to image the cellular uptake by HMMs and distribution of chemically modified MWNTs we used 3-D dark-field scanning transmission electron microscopy tomography of freeze-dried whole cells and scanning electron microscopy. [1] C. Cheng, K. H. Müller, K. K. K. Koziol, J. N. Skepper, P. A. Midgley, M. E. Welland, A. E. Porter, Biomaterials, 2009, 30, 4152.

### Exploring bio-functionalized CNTs and their interaction with cells using atomic force and fluorescence microscopy

**Constanze Lamprecht**, *Johannes Kepler University Linz, Austria* | **Birgit Plochberger**, *Johannes Kepler University Linz, Austria* | **Elena Heister**, *University of Surrey, UK* | **Michael Leitner**, *Johannes Kepler University Linz, Austria* | **Ivan Liashkovich**, *Institute of Physiology II, Germany* | **Petar Lukanov**, *Centre Interuniversitaire de Recherche et d'Ingénierie des Matériaux, Toulouse* | **Emmanuel Flahaut**, *Centre Interuniversitaire de Recherche et d'Ingénierie des Matériaux, Toulouse* | **Ferry Kienberger**, *Agilent Laboratories Linz, Austria* | **Andreas Ebner**, *Johannes Kepler University Linz, Austria* | **Peter Hinterdorfer**, *Johannes Kepler University Linz, Austria*

At present, the atomic force microscope (AFM) offers a unique solution to study biological specimens on the nanometer scale under (near-) physiological conditions without the need for rigorous sample preparation, staining or labelling. We expected new and significant bio-physical insights into the delivery process and transport mechanism of CNTs into cells employing the AFM. Here we give an overview for the application of AFM to characterize and assess CNT surface bio-functionalization. We present the new and emerging technique of simultaneous topographical and recognition (TREC) to directly visualize functionality of biomolecules attached to CNTs under physiological conditions. Moreover, we show how topographic AFM imaging can be used to study the binding of functionalized single walled carbon nanotubes (SWNT), double walled carbon nanotubes (DWNT) and multi walled carbon nanotubes (MWNT) to various relevant biological membranes, including nuclear membranes and cell surfaces. Current experiments involve the combination of fluorescence and atomic force microscopy to localize binding of functionalized carbon nanotubes to cell surfaces. These preliminary studies will facilitate the investigation of the binding of fluorescently labelled CNTs to the cell and their possible internalization in a time resolved manner. We show first results of uptake experiments, where we were able to trace individual carbon nanotubes internalized into living cells.

### Impact of In Vitro Exposure to Carbon Nanotube on Molecular Changes at Cellular Level

**Premkumari Kumarathasan**, *Safe Environments Programme, Health Canada, Canada* | **Dharani Das**, *Safe Environments Programme, Health Canada, Canada* | **Dalibor Breznan**, *Safe Environments Programme, Health Canada, Canada* | **Anu Saravanamuthu**, *Safe Environments Programme, Health Canada, Canada* | **Agnieszka Bielecki**, *Safe Environments Programme, Health Canada, Canada* | **Susantha Mohottalage**, *Safe Environments Programme, Health Canada, Canada* | **Erica Blais**, *Safe Environments Programme, Health Canada, Canada* | **Benoit Simard**, *Safe Environments Programme, Health Canada, Tunney's Pasture,Canada* | **Renaud Vincent**, *Safe Environments Programme, Health Canada, Canada*

Tracking proteomic and metabolite changes can be valuable in obtaining information on free radical-mediated modifications and protein profile changes caused by pollutant exposure-induced effects. Here, we have compared the biological effects induced by exposure to four types of carbon-based particles in the J774 murine macrophage cell line: single-walled and multi-walled pristine and oxidatively-modified carbon nanotubes (CNT). Cells were exposed to the particles at 0-100 ìg/cm2 (96-well plates) in serum-free medium for 24h. Physico-chemical characteristics of carbon nano materials were conducted. Cell lysates and supernatants were analyzed for oxidatively modified protein metabolites by a HPLC-coulometric array detection method. Whereas, shotgun proteomic analyses of cell lysates were then performed by direct MALDI-TOF-TOF-MS after sample clean up. Saturated alpha-cyano-4-hydroxycinnamic acid served as the matrix. The mass spectral profiles were interrogated in the region <6kDa using k-nearest neighbor clustering algorithm. Our results clearly indicated that J774 cells exposed to these particles exhibited characteristic mass spectral profiles. Also, the MS data revealed dose related elevation of cellular endothelin-1 peptide in J774 cells a descriptor of inflammatory status of macrophages. Association of physicochemical characteristics of these particles with induced biological changes provide new insights into mechanisms of particle toxicity.

### Carbon nanotubes as drug delivery systems: Material-related problems and how to solve them

**Elena Heister**, *University of Surrey, Guildford, UK* | **V. Neves**, *Faculty of Health and Medical Sciences, University of Surrey; Nanoelectronics Centre, Advanced Technology Institute, University of Surrey* | **H. M. Coley**, *Faculty of Health and Medical Sciences, University of Surrey* | **S. R. P. Silva**, *Nanoelectronics Centre, Advanced Technology Institute, University of Surrey* | **J. McFadden**, *Faculty of Health and Medical Sciences, University of Surrey*

Aqueous dispersions of functionalized carbon nanotubes (CNTs) are widely used for biomedical applications, such as drug delivery, gene delivery, or cellular/in vivo imaging. The dispersion stability of such preparations, however, depends on a wide range of parameters, such as length, aspect ratio, surface charge, and functionalization of the nanotubes, as well as pH and composition of the surrounding medium. We have undertaken an extensive study to understand how these factors can be tuned in order to obtain an optimal dispersion stability of carbon nanotubes in chemical and biological environments. Furthermore, we have been able to demonstrate that a carbon nanotube-based delivery system for anticancer drugs loses its therapeutic efficacy, if the dispersion stability is poor. Another material-related problem for the use of oxidized carbon nanotubes as drug delivery systems is the generation of oxidation debris during the acid oxidation process. Previous studies have mainly focused on the characterisation of this debris and how to remove it, as it can present a pitfall for effective covalent functionalization of CNTs (which is likely to occur at the level of the debris and not the actual CNT surface). We went a step further and investigated the effect of present oxidation debris on the drug delivery properties of carbon nanotubes. Preliminary results indicate that oxidation debris has a much higher capability to transport drug molecules inside cancer cells than carbon nanotubes, comparable to oxidised graphene.

## Trapping of spherical and elongated magnetic particles in microfluidic systems

**Kirsten Pondman**, *Low Temparature Division, MIRA Institute, University of Twente, Enschede, The Netherlands* | **Martin Sobik**, *Low Temparature Division, MIRA Institute, University of Twente, Enschede, The Netherlands* | **Shashank Shekhar**, *Nanobiophysics, MESA+ Institute for Nanotechnology & MIRA University of Twente, The Netherlands* | **Severine le Gac,** *BIOS the Lab-on-a-Chip group, MESA+ Institute for Nanotechnnology, University of Twente, The Netherlands* | **Silke Hampel**, *Leibniz-Institute for Solid State and Materials Research, Germany* | **Horst Rogalla**, *Low Temparature Division, MIRA Institute, University of Twente, Enschede, The Netherlands* | **Bennie ten Haken**, *Low Temparature Division, MIRA Institute, University of Twente, Enschede, The Netherlands*

Magnetic manipulation of particles in microfluidic systems has been applied only recently. Magnetic forces can be used for transport, positioning, separation and sorting of magnetic particles and magnetically tagged cells and e.g. proteins. Most commonly magnetic nanoparticles in microfluidics serve as a surface for bio- or immunoassays, which can therefore be done in a small volume and very localised [1]. In this study magnetic trapping of commonly used spherical superparamagnetic particles (Endorem) and elongated nanoparticles, Fe-filled multi walled carbon nanotubes (Fe-MWNTs) is studied. Suspensions of both types of particles are in a microfluidic chip and trapping is achieved by the use of a magnetic needle with a high gradient magnetic field (7500 T/m). Although the mass magnetization of Endorem is a factor ten higher compared to the Fe-MWNTs due to the low filling grade of the nanotubes trapping is still possible. Furthermore Fe-MWNTs have potential in lab-on-a-chip-devices thanks to there large surface area for binding of proteins etc. 1. Pamme, N., Magnetism and microfluidics. Lab on a Chip, 2006. 6(1): p. 24-38

## Confocal microscopic study of diameter dependent delivery of siRNA into|keratinocytes by multiwall carbon nanotubes

**Evi Saliaj**, University of Waterloo | **Mahmoud Elsabahy**, University of Waterloo | **Marina Ivanova**, University of Waterloo | **Marianna Foldvari**, University of Waterloo

Cutaneous gene therapy requires the successful delivery of nucleic acids (plasmid DNA or RNA) into keratinocytes in the epidermis and modulation of both local and systemic effects. We examined the effect of diameter of multiwall carbon nanotubes (MWNT) on the efficiency and toxicity of siRNA delivery in PAM212 keratinocytes. MWNTs with outer diameters of 15nm, 30nm, 40nm or 50nm were non-covalently functionalized with 0.1% aqueous dicationic 12-3-12 surfactant. siGLO-RNA was attached to the MWNTs (0.01mg/mL) by non-covalent binding. Control formulations included MWNTs dispersed in water, surfactant alone, siGLO-RNA alone and no treatment. MWNTs were characterized by centrifugation, UV spectrometry and transmission electron microscopy (TEM). PAM212 keratinocytes (1million/3mL MEM) were plated in 3cm MatTek Petri dishes and dosed with 0.705µg of siGLO-RNA/100&#61549;L. The uptake and fate of siGLO-RNA (Lambda ex=543/Lambda em=570) was followed using a Zeiss710 confocal microscope for 24h. Cells were co-stained with calcein (Lambda ex=488/Lambda em=520) as an indicator of cell viability and DRAQ5 (Lambda ex=633/ Lambda em=670) nuclear stain. TEM study showed individually dispersed nanotubes and nanoscale structural differences among different diameter MWNTs. Generally, transfection increased significantly after 6h and continued up to 24h for all MWNTs. MWNTs functionalized with 12-3-12 surfactant were more effective in cell transfection as compared to MWNTs dispersed in water. The highest transfection levels were achieved with MWNT15. Transfection efficiency decreased with increasing nanotube diameter. Cell viability decreased after treatment with surfactant-functionalized siRNA-MWNTs by 46% and by 67% with surfactant alone compared to untreated cells. This study showed a correlation between siRNA delivery into keratinocytes and MWNT diameter.

## Detection of single-molecule H2O2 signalling from epidermal growth factor receptor using fluorescent single-walled carbon nanotubes

**Hong Jin**, *Massachusetts Institute of Technology, USA* | **Jingqing Zhang**, *Massachusetts Institute of Technology, USA* | **Hyeonseok Yoon**, *Massachusetts Institute of Technology, USA* | **Michael Strano**, *Massachusetts Institute of Technology, USA*

An emerging concept in cell signalling is the natural role of reactive oxygen species such as hydrogen peroxide (H2O2) as beneficial messengers in redox signalling pathways. In spite of the growing evidence, the nature of H2O2 signalling is confounded by difficulties in tracking it in living systems, both spatially and temporally, at low concentrations. Here, we develop an array of fluorescent single-walled carbon nanotubes that can selectively record, in real time, the discrete, stochastic quenching events that occur as H2O2 molecules are emitted from individual human epidermal carcinoma cells stimulated by epidermal growth factor.(Jin, et al. 2008; Jin, et al. 2010) We show mathematically that such arrays can distinguish between molecules originating locally on the cell membrane from other contributions. We find that epidermal growth factor induces 2 nmol H2O2 locally over a period of 50 min. This platform promises a new approach to understanding the signalling of reactive oxygen species at the cellular level. Jin, H., et al. (2010). 'Detection of single-molecule H2O2 signalling from epidermal growth factor receptor using fluorescent single-walled carbon nanotubes.' Nature Nanotechnology (Submitted). Jin, H., et al. (2008). 'Stochastic analysis of stepwise fluorescence quenching reactions on single-walled carbon nanotubes: single molecule sensors.' Nano letters 8(12): 4299-4304.

# 1st Graphene Satellite Symposium (GSS10)

**Organizers:**
**Antonio H. Castro Neto**, *Department of Physics, Boston University, USA*
**Alexander Grüneis**, *Faculty of Physics, Universitat Wien, Austria*
**Tony F. Heinz**, *Department of Physics & Department of Electrical Engineering, Columbia University, USA*
**Thomas Szkopek**, *Department of Electrical and Computer Engineering, McGill University, Canada)*

## ROOM: MONT-ROYAL

## Sunday, June 27

### 8:30-8:40

**Welcoming Remarks**
**Thomas Szkopek**

### ■ *Introduction to Graphene*

### 8:40-9:20 Invited Speaker

**Theoretical Aspects of Graphene Physics**
**Antonio Castro Neto**, *Department of Physics, Boston University, USA*

Graphene is an unusual material in many respects. Because graphene is one atom thick, metallic, and has exotic electronic excitations in the form of Dirac quasiparticle, its theoretical description brings together topics from quantum relativistic physics, soft and hard condensed matter. In this tutorial we will review some of the most important theoretical topics in graphene and discuss their experimental consequences.

### 9:20-10:00 Invited Speaker

**Electron-Electron Interactions in Graphene**
**Philip Kim**, *Columbia University, USA*

Electrons confined in two dimensions (2D) can exhibit strongly correlated states. Recent experimental discovery of integer and fractional quantum Hall effect in graphene amplified interest in correlated 2D electronic systems, owning to presence of the unusual topological phase associated with zero effective mass of charge carriers. In this talk, we will discuss the transport, employing both Hall bar geometry samples and Corbino geometry samples, and infrared spectroscopy results that reveal the role of the many-body effects due to the electron-electron interaction in graphene near the Dirac point. In particular, we will discuss the unusual spontaneous symmetry breaking of single particle LLs under the extreme quantum condition in single and bilayer graphene together with the appearance of unique low density insulating states and fractional quantum Hall states.

### Coffee Break / Posters

### ■ *Graphene Chemistry and Structure*

### 10:20-11:00 Invited Speaker

**Graphene and Its Chemical Derivatives**
**Kostya Novoselov**, *University Of Manchester, United Kingdom*

Extraordinary properties of graphene continue to attract intense interest that has expanded into research areas beyond the initial studies of graphene's electronic properties. One of the research directions that have emerged recently is based on the notion of graphene being a giant macromolecule that as any other molecule can be modified in chemical reactions. Particularly enticing is the possibility to create stoichiometric graphene-based derivatives such as, for example, graphene rather than to simply decorate graphene's surface with various atoms and molecules. I will report on fully fluorinated graphene (fluorographene), which is made by exposure of both surfaces of suspended graphene to atomic fluorine. This stable insulating counterpart of graphene expands the range of possibilities offered by graphene itself, allowing the latter to be (locally) modified to meet specific demands in, for example, electronic and optoelectronic applications.

### 11:00-11:40 Invited Speaker

**Control of Graphene's Properties by Reversible Hydrogenation: Evidence for Graphene**
**Daniel C. Elias**, *The University Of Manchester, United Kingdom* | **R. R. Nair**, *The University Of Manchester, United Kingdom* | **T. M. G Mohiuddin**, *The University Of Manchester, United Kingdom* | **S. V. Morozov**, *Institute for Microelectronics Technology, Russia.* | **P. Blake**, *Manchester Centre for Mesoscience and Nanotechnology, University of Manchester, UK.* | **M. P. Halsall**, *The University Of Manchester, United Kingdom* | **A. C. Ferrari**, *Department of Engineering, Cambridge University, UK* | **D. W. Boukhvalov**, *Institute for Molecules and Materials, Radboud University Nijmegen, Netherlands* | **M. I. Katsnelson**, *Institute for Molecules and Materials, Radboud University Nijmegen, Netherlandss* | **A. K. Geim**, *The University Of Manchester, United Kingdom* | **K. S. Novoselov**, *The University Of Manchester, United Kingdom*

Although graphite is known as one of the most chemically inert materials, we have found that graphene, a single atomic plane of graphite, can react with atomic hydrogen, which transforms this highly conductive zero-overlap semimetal into an insulator. Transmission electron microscopy reveals that the obtained graphene derivative (graphane) is crystalline and retains the hexagonal lattice, but its period becomes markedly shorter than that of graphene. The reaction with hydrogen is reversible, so that the original metallic state, the lattice spacing, and even the quantum Hall effect can be restored by annealing. Our work illustrates the concept of graphene as a robust atomic-scale scaffold on the basis of which new two-dimensional crystals with designed electronic and other properties can be created by attaching other atoms and molecules.

### 11:40-12:00 Contributed Talk

**Ultraflat graphene**
**Chun Hung Lui**, *Columbia University, USA* | **Li Liu**, *Columbia University, USA* | **Kin Fai Mak**, *Columbia University, USA* | **George W. Flynn**, *Columbia University, USA* | **Tony F. Heinz**, *Columbia University, USA*

Much of the research on graphene has been directed towards exploration of its novel electronic properties, but the structural aspects of this model two-dimensional system are also of great interest. In particular, microscopic corrugations have been observed on all suspended and supported graphene sheets studied so far. Many distinctive electronic and chemical properties of graphene have been attributed to the presence of such ripples, which are also predicted to give rise to new physical phenomena that would be absent in a planar two-dimensional material. Direct experimental study of such novel ripple physics has, however, been hindered by the lack of flat graphene layers. Here we report the fabrication of graphene monolayers that are flat down to the atomic level. The samples are produced by deposition on the atomically flat terraces of cleaved mica surfaces. The apparent height variation in the graphene layers observed by high-resolution atomic force microscopy (AFM) is less than 25 pm, indicating the suppression of any existing intrinsic ripples in graphene. The availability of such ultraflat samples should facilitate rigorous testing of the impact of ripples on various physical and chemical properties of graphene.

## Lunch / Posters

## ■ *Graphene Electronic Properties I*

### 13:20-14:00 Invited Speaker

**Recent Development of Gigahertz Graphene FETs**
**Yu-Ming Lin**, *IBM T. J. Watson Research Center, USA*

The recent excitement about graphene as a possible material for high-frequency electronics has lead to demonstrations of high-frequency field-effect transistors (FETs) in the last two years. Although graphene FETs operate by a different principle than silicon MOSFETs, and have different dc characteristics, their ac characteristics are quite similar. Hence the high intrinsic mobility of graphene leads to the expectation of high frequency operation of gated graphene FETs. Demonstrations of frequency response in the GHz regime have been shown using both exfoliated flakes and synthesized graphene. Here we review recent experimental progress and modeling development of graphene FETs for high-frequency electronics. By improving the oxide deposition process an intrinsic cut-off frequency as high as 100 GHz has been achieved in a 240-nm-gate graphene FET fabricated on a 2" wafer of epitaxially grown graphene. This fT value exceeds that of Si MOSFETs at the same gate length, illustrating the potential of graphene for RF applications. Co-workers: K. Jenkins, D. Farmer, C. Dimitrakopoulos, H.-Y. Chiu, A. Valdes-Garcia, A. Grill, and P. Avouris.

### 14:00-14:40 Invited Speaker

**Tunable electronic properties of functionalized graphene studied by photoemission spectroscopy**
**Alexander Grueneis**, *IFW Dresden And University Of Vienna, Germany*

Ionic and covalent functionalization are key to tune graphene's electronic properties. Here we perform functionalization of chemical vapour deposition (CVD) grown graphene monolayers with alkali and hydrogen atoms. This allows for tuning both, the energy gap and the electron concentration independently, which is a prerequisite for device applications. The chemical bonding and the concentrations of the adsorbed atoms are determined with high accuracy using core level and x-ray absorption spectroscopies. Angle-resolved photoemission spectroscopy provides access to the electron-phonon coupling and a peculiar localized state hydrogenated graphene which is governed by the electron density. We show results on the dependence of the electron phonon coupling on doping level, wavevector direction and the impurity concentration. Finally, the metal insulator transition in graphene is discussed in terms of band insulator versus electron localization.

### 14:40-15:00 Contributed Talk

**Local Electronic Properties of Graphene**
**Brian LeRoy**, *University of Arizona, USA* | **Aparna Deshpande**, *University of Arizona, USA* | **Daniel Cormode**, *University of Arizona, USA* | **Wenzhong Bao**, *University of California Riverside* | **Feng Miao**, *University of California Riverside* | **Zeng Zhao**, *University of California Riverside* | **Jeanie Lau**, *University of California Riverside*

Combining scanning probe microscopy with electrical transport measurements is a powerful approach to probe low-dimensional systems. The local information provided by scanning probe microscopy is invaluable for studying effects such as electron-electron interactions and scattering. Using this approach, we have probed the local electronic properties of mono- and bilayer graphene with atomic resolution using scanning tunneling spectroscopy. We studied the effect of ripples, charged impurities and defects on the local density of states. We find that long-range scattering from charged impurities locally shifts the Dirac point leading to electron and hole puddles. These puddles are not correlated with the topography and therefore are not due to ripples. Recent measurements are able to spatially localize individual charged impurities and understand their effect on the density of states. We have also observed short-range scattering from lattice defects that mixes the two sublattices of graphene and tends to be strongly suppressed away from the Fermi energy. In addition, in bilayer graphene we observe an opening of a band gap and controlled shift of the Dirac point due to the application of a transverse electric field.

## Coffee Break / Posters

## ■ *Graphene Electronic Properties II*

### 15:20-16:00

**Air Doping of Graphene on SiO2: the Mechanism**
**Pierre L. Levesque**, *Université de Montréal, Canada* | **Shadi Sabri**, *McGill University* | **Carla M. Aguirre**, *École Polytechnique de Montréal* | **Jonathan Guillemette**, *McGill University* | **Mohamed Siaj**, *Université du Québec à Montréal* | **Patrick Desjardins**, *École Polytechnique de Montréal* | **Thomas Szkopek**, *McGill University* | **Richard Martel**, *Université de Montréal, Canada*

Graphene field effect transistor (FET) are p-doped in air. Undoped and even n-doped graphenes have however been observed under certain conditions, for instance when graphene devices have been annealed in vacuum. To explain this behaviour, widely-held views are that graphene is p-doped by atmospheric adsorbates or by impurities. In the present study, we investigated the influence of gas adsorbates on the transfer characteristics of graphene FETs having different types of gate dielectrics. Our study revealed that graphene FET on hydrophilic silicon dioxide substrates is not affected by exposure to dry O2 or N2 and readily n-doped by water. In contrast, the FET devices on hydrophobic gate dielectric substrates are unaffected in air[1]. A p-doping effect is only seen for the devices on SiO2 when exposed simultaneously to both O2 and water. We therefore propose that the underlying phenomenon behind the effective doping of graphene devices is due to an electrochemical charge transfer reaction between the graphene and the oxygen-water redox couple. These findings reinforce our belief that redox active species directly influence the transport properties of graphene transistors in air. A general mechanism is proposed to explain this doping behaviour. [1] S. S. Sabri et al., Applied Physics Letters 95, 242104 (2009).

### 16:00-16:40 Invited Speaker

**Electronic Transport in Bilayer Graphene**
**Pablo Jarillo-Herrero**, *Massachusetts Institute of Technology, USA*

I will discuss our recent experiments on electronic transport in dual-gated bilayer graphene.

## ■ *Graphene Theory*

### 16:40-17:20 Invited Speaker

**On-demand Engineering of Electronic Transport in Graphene**
**Vitor Pereira**, *Boston University, USA* | **Antonio Castro Neto**, *Boston University, USA* | **Nuno Peres**, *Universidade do Minho (Portugal)*

Graphene is currrently the most flexible material for nanoscale applications. Being a monoatomic surface, the entire system is exposed to the environment and readily amenable for various kinds of interaction and manipulation. The fast pace of development in synthesis and fabrication, are bringing the concept of 'tunability on demand' to the verge of reality in graphene. This concept entails the ability to manipulate electronic and transport properties of devices in a controlled, and reversible way, not only during the fabrication stage, but also in real time for operational devices. In this context I will discuss possible routes to achieve such tunability under the light of recent results on the interplay between electronic and structural degrees of freedom.

The fact that graphene is not only remarkable electronically, but also mechanically (featuring the largest Young modulus ever measured, and sustaining elastic deformations in excess of 20%), makes the interplay between structure and electronics an entirely new avenue of research, not frequently available in conventional materials. As some examples, I will show how adequate clamping conditions can lead to selective adsorption of chemical species to graphene; how planar strain affects its electronic structure; how local strain profiles can generate local reversible confinement and quantization, without lithography; and how extrinsic tunable wrinkles might be used to manipulate the mobility.

## 17:20-18:00 Poster

### Theoretical Issues of the Fractional Quantum Hall Effect in Graphene

**Mark Oliver Goerbig**, *CNRS, University Paris Sud, France*

Graphene in a strong magnetic field may be viewed as a four-component quantum Hall system, as a consequence of its four-fold spin-valley degeneracy that governs the low-energy electronic properties. Whereas the integer quantum Hall regime is strongly affected by the relativistic character of the massless carriers in graphene and yields the so-called relativistic quantum Hall effect, the fractional quantum Hall effect and other strongly-correlated electronic phases in a partially filled Landau level are essentially non-relativistic. However, the four-component character survives and is respected to great accuracy by the physically relevant Coulomb interaction. We investigate the graphene fractional quantum Hall effect, some states of which have recently been observed experimentally in a two-terminal transport measurement on suspended samples, within the framework of multi-component wave functions.

## 18:00-18:20

### Novel broken-symmetry ground states in bilayer graphene

**René Côté**, *Université De Sherbrooke, Canada* | **Jules Lambert**, *Université De Sherbrooke, Canada* | **Yafis Barlas**, *NHMFL and Florida State University* | **Allan H. MacDonald**, *University of Texas at Austin*

In this work, we present a study of the two-dimensional electron gas (2DEG) in a graphene bilayer in a quantizing magnetic field. We focus on filling factors -1 and -3 i.e. on states within the octet of degenerate states of the N=0 Landau level. We show that the electron interaction leads to novel broken-symmetry states with transport properties that can be very different from those found in conventional semiconductor bilayers. For example, the ground state at -3 has spontaneous interlayer coherence and a pseudospin mode that has quadratic rather than the expected linear dispersion. It follows that the superfluid density of the exciton condensate vanishes. We also find that any finite potential difference between the graphene layers makes the state unstable and induce, via thermal fluctuations, a first order isotropic-smectic phase transition. At filling factor -1, the state at zero bias also has interlayer coherence. With applied bias, however, there is a transition to a phase with "orbital" coherence. This type of coherence is specific to bilayer graphene where both n=0 and n=1 orbital Landau levels have zero kinetic energy. If we associate an "orbital" pseudospin with these two levels, this new ground state can be described as a quantum Hall "orbital ferromagnetic state". This liquid state has a finite density of electric dipoles and an extra Goldstone mode with a highly anisotropic dispersion. The effective pseudospin wave model that describes this state has a Dzyaloshinskii-Moriya term that leads to the formation of a ground state with spiral orbital-pseudospin order.

# 1st Graphene Satellite Symposium (GSS10)

## ROOM: MONT-ROYAL

## Monday, June 28

### ■ *Graphene Electronic Properties III*

#### 8:40-9:20 Invited Speaker

**Evolution of Dirac fermions in various graphene structures**
**Shuyun Zhou**, *Lawrence Berkeley National Lab, USA* | **Alessandra Lanzara,** *Department of Physics, UC Berkeley; Materials Sciences Division, Lawrence Berkeley National Lab*

I will present our study of the electronic structure of various graphene samples including epitaxial graphene, exfoliated graphene and graphene nanostructures using spectroscopic and microscopic techniques. I will discuss about what drives the stability of graphene from the comparison between epitaxial and exfoliated graphene. I will also discuss the effects of many-body interactions, doping, nanometer terrace size on the electronic properties and the implications of these results.

#### 9:20-10:00 Invited Speaker

**Electronic Structure and Magnetic Properties of Noble-Metal-Intercalated Graphene on Ni(111)**
**Andrei Varykhalov**, *Helmholtz-Zentrum Berlin, Germany* | **Dmitry Marchenko**, *Helmholtz-Zentrum Berlin, Germany* | **Markus Scholz,** *Helmholtz-Zentrum Berlin, Germany* | **Timur Kim**, *IFW-Dresden, Germany* | **Oliver Rader**, *Helmholtz-Zentrum Berlin, Germany*

Graphene is among the most promising materials for future electronic devices. It features both interesting charge and spin transport properties such as quasirelativistic charge carriers with vanishing mass and efficient spin injection and spin transport. In the context of device fabrication a controllable energy gap is required at the Fermi level, but graphene grown on SiC is n-doped with the Dirac point below the Fermi energy. In our experiments we have achieved quasifreestanding graphene on metallic substrates. Its electronic properties are very close to the those of ideal graphene. Graphene is synthesized on Ni(111) by chemical vapor deposition. After intercalation of Au between the graphene and Ni substrate, the initially strong C-Ni interaction is blocked and the linear relativistic dispersion of freestanding gapless and undoped graphene is recovered. When the Au interlayer is replaced by Cu or Ag, the graphene becomes n-doped with an energy shift comparable to recent DFT calculations, but the contact to Ag or Cu is found to open a substantial bandgap in the graphene. For the Au-intercalated graphene, we observe by spin-resolved photoemission a large Rashba-type spin-orbit splitting of the pi-state. The splitting is by three orders of magnitude larger than expected for pure graphene and assigned to the influence of the Au underneath and its large atomic number. In addition, we demonstrate that quasifreestanding graphene on Au is a chemically passive system: its electronic structure remains completely unaffected by exposure to atmosphere.

#### Coffee Break / Posters

### ■ *Graphene Magnetic Properties*

#### 10:20-11:00 Invited Speaker

**Quantum Resistance Standard Based on Epitaxial Graphene**
**Samuel Lara-Avila**, *Chalmers University Of Technology, Sweden* | **Sergey Kubatkin**, *Chalmers University Of Technology, Sweden* | **Alexander Tzalenchuk**, *National Physical Laboratory, UK* | **Alexei Kalaboukhov**, *Chalmers University Of Technology, Sweden* | **Sara Paolillo**, *Politecnico di Milano, Italy* | **Mikael Syvajarvi**, *Linkoping University, Sweden* | **Rosiza Yakimova**, *Linkoping University, Sweden* | **Olga Kazakova**, *National Physical Laboratory, UK* | **Jan-Theodoor Janssen**, *National Physical Laboratory, UK* | **Vladimir Fal'ko**, *Lancaster University, UK*

We report development of a quantum Hall effect (QHE) resistance standard accurate to a few parts in a billion and based on large area graphene produced on silicon carbide [1]. Graphene was grown at 2000°C and 1 atm Ar gas pressure, which resulted in monolayers of graphene atomically uniform over more than 50 µm^2. Hall bars 2-35 µm wide and 11-160 µm long were produced using standard electron beam lithography and oxygen plasma etching. The manufactured material was n-doped, due to charge transfer from SiC, with the measured electron concentration in the range of (5-10)x10^11 cm^-2, mobility about 2400 cm^2/Vs at room temperature and between 4000 and 7500 cm^2/Vs at 4.2 K. A polymer layer on top of graphene resulted in better sample temporal stability, higher uniformity, reduced electron density and significantly improved electron mobility. Transport measurements and atomic force microscopy show that the graphene layer covered the substrate steps preserving its structural integrity. Magnetotransport measurements revealed a sequence of Hall plateaux characteristic for single-layer graphene. Precise measurements performed using a cryogenic current comparator showed robust quantum Hall quantization on nu=2 plateau accurate to some parts per billion over a few Tesla, tens of microampere and tens of Kelvin. We believe that the new results on graphene will help expand the horizon of quantum metrology and advance the understanding of both graphene and QHE. References [1] A Tzalenchuk et al., Nature Nanotechnology 5, 186 (2010).

#### 11:00-11:40 Invited Speaker

**Magnetism and STM spectroscopy on graphene**
**Bruno Uchoa**, *University Of Illinois At Urbana-Champaign, USA*

As an open surface, the use of scanning tunneling microscopy (STM) probes in graphene opens the possibility of controlling the position of adatoms with atomic precision and at the same time switching the magnetic local moments on and off by gating [1]. For a disordered distribution of magnetic adatoms, the interplay of the RKKY interaction and the correlation induced by the ripples can generate a variety of macroscopic magnetic states, with distinctive signatures in magnetoresistance and in the magnetization [2]. After addressing the Anderson impurity model in graphene, which describes the formation of local magnetic moments in magnetic adatoms with inner shell electrons, I will show how STM probe measurements can be used to detect local magnetism in graphene, taking advantage of the low density of states and of quantum interference effects naturally inbuilt in the honeycomb lattice structure [3]. [1] B. Uchoa et. al., Phys. Rev. Lett. 101, 026805 (2008) [2] T. G. Rappoport, B. Uchoa, and A. H. Castro Neto, Phys. Rev. B 80, 245408 (2009) [2] B. Uchoa et. al. , Phys. Rev. Lett. 103, 206804 (2009).

#### 11:40-12:00 Contributed Talk

**Cyclotron resonance near the charge neutrality point of graphene**
**Zhigang Jiang**, *Georgia Institute Of Technology, USA* | **Erik Henriksen,** *California Institute of Technology* | **Paul Cadden-Zimansky**, *Columbia University; National High Magnetic Field Laboratory* | **Li-Chun Tung**, *National High Magnetic Field Laboratory* | **Yong-Jie Wang**, *National High Magnetic Field Laboratory* | **Philip Kim**, *Columbia University* | **Horst Stormer**, *Columbia University; Bell Labs*

Due to the unusual dispersion relation and non-zero Berry's phase of its charge carriers, the Landau level (LL) spectrum that forms in graphene when it is subjected to a magnetic field exhibits a number of distinctive features. In addition to an uneven spacing of the levels, the most notable feature is the formation of an 'n=0' LL at the charge-neutrality point, where the carriers switch from holes to electrons. While the lack of a zero in the longitudinal resistance precludes some of the traditional methods for characterizing the n=0 LL through edge state conductance, the bulk properties of this level can be directly probed by examining the cyclotron resonance (CR) transitions into and out of this level. By measuring the infrared absorption of graphene in high fields, we track the evolution of these absorption energies as the Fermi level is gradually tuned through the charge-neutrality point. Though the interband transitions from n=-1 -> 2 and n=-2 -> 1 exhibit no change in CR energy as the Fermi level is changed, large shifts (~15 meV at 18 T) are observed in the absorption energy for transitions into and out of the n=0 LL in both single-layer and bilayer graphene. While the shift of the CR of single-layer graphene evolves non-monotonically with respect to filling factor, the analogous bilayer shift increases monotonically. In particular, the resonance evolution in single-layer graphene is indicative of a field-dependent energy gap opening at the Dirac point.

### Lunch / Posters

## ■ *Graphene Optical Properties I*

### 13:00-13:40 Contributed Talk

**Graphene photonics: ultrafast lasers and photoluminescence**
**Andrea C. Ferrari**, *University of Cambridge, UK*

The richness of optical and electronic properties of graphene attracts enormous interest. So far, the main focus has been on fundamental physics and electronic devices. However, we believe its true potential to be in photonics and optoelectronics, where the combination of its unique optical and electronic properties can be fully exploited, the absence of a bandgap can be beneficial, and the linear dispersion of the Dirac electrons enables ultra-wide-band tunability. The rise of graphene in photonics and optoelectronics is shown by several recent results, ranging from solar cells and light emitting devices, to touch screens, photodetectors and ultrafast lasers. Despite being a single atom thick, graphene can be optically visualized [1]. Its transmittance can be expressed in terms of the fine structure constant [2]. The linear dispersion of the Dirac electrons enables broadband applications. Saturable absorption is observed as a consequence of Pauli blocking [3,4]. Chemical and physical treatments enable luminescence [5]. Graphene-polymer composites prepared using wet chemistry [3-5] can be integrated in a fiber laser cavity, to generate ultrafast pulses, down to 200fs, and enable broadband tunability [3,4]. [1] C. Casiraghi et al. Nano Lett. 7, 2711 (2007). [2] R. R. Nair et al. Science 320, 1308 (2008). [3] T. Hasan, et al. Adv. Mat. 21,3874 (2009) [4] Z. Sun et al. ACS Nano 4, 803 (2010); arxiv 1002.0653v1 (2010) [5] T. Gokus et al. ACS nano 3, 3963 (2009)"

## ■ *Large Area Graphene*

### 13:40-14:20 Invited Speaker

**Self-standing Graphene Sheets prepared with Chemical Vapor Deposition and Chemical Etching**
**Genki Odahara**, *Waseda University, Japan* | **Tsuyoshi Ishikawa**, *TOYOTA central laboratory* | **Shigeki Otani**, *National Institute for Material Science* | **Chuhei Oshima**, *Waseda University*

On a Ni (111) surface, a single-layer graphene sheet with a 1 x 1 atomic structure grew up in epitaxial way. Chemical etching the substrate made it possible to separate macroscopic self-standing sheets of graphene a few tenth mm in size, which were characterized by transmission electron microscopy (TEM).

### 14:20-15:00 Invited Speaker

**Epitaxial graphene on SiC: controlling the growth, electronic and structural properties**
**Konstantin Emtsev**, *Max Planck Institute For Solid State Research, Germany* | **Thomas Seyller**, *Chair of Technical Physics, University Erlangen-Nuremberg* | **Lothar Ley**, *Chair of Technical Physics, University Erlangen-Nuremberg* | **Ulrich Starke**, *Max Planck Institute For Solid State Research, Germany*

Growth of graphene on silicon carbide (SiC) is considered among the most promising methods for large scale graphene production [1]. Especially, use of insulating single crystal SiC wafers allows a direct application of graphene on SiC in electronics. This, however, requires a uniform, ordered growth of graphene thin films as well as detailed understanding and control of their structure and interface properties. These are the topics of the present talk. In particular, we will discuss a furnace growth method introduced recently [2] which results in monolayer graphene films with significantly improved morphology and homogeneity. Epitaxial graphene layers were produced on the SiC surfaces by solid-state decomposition at elevated temperatures in argon atmosphere. An extensive characterization of the atomic, structural and electronic properties of the grown graphene films and their interfaces with SiC substrate was carried out by low-energy electron diffraction (LEED), low-energy electron microscopy (LEEM), angle-resolved photoelectron spectroscopy (ARPES), X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy. In addition, several strategies which allow us to modify the electronic properties of the as-grown epitaxial graphene such as fabrication of quasi-free standing graphene on SiC [3] will be discussed. [1] W.A. de Heer, Solid State Communications 143, 92 (2007). [2] K.V. Emtsev et al., Nature Materials, 8, 203 (2009). [3] C. Riedl et al., Phys. Rev. Lett. 103, 246804 (2009).

### Coffee Break / Posters

## ■ *Graphene Optical Properties II*

### 15:20-16:00 Invited Speaker

**Observation of Plasmarons in Doped Quasi-Freestanding Graphene**
**Aaron Bostwick**, *Lawrence Berkeley National Lab*

Graphene is a remarkable new electronic material with many unique properties. To realize its promise, it is essential to understand how its charge carriers interact. By measuring the spectral function of charge carriers in quasi-free-standing graphene, we show that at finite doping, the well-known linear Dirac spectrum does not provide a full description of the charge-carrying excitations. We report that there also exist composite 'plasmaron' particles, consisting of particles bound to density oscillatons of the graphene electron gas. The Dirac crossing point is resolved into three crossings: the first between pure charge bands, the second between pure plasmaron bands, and the third a ring-shaped crossing between charge and plasmaron bands.

### 16:00-16:40 Invited Speaker

**Optical spectroscopy of graphene and multilayer graphene**
**Zhiqiang Li**, *Columbia University, USA* | **Dimitri Basov**, *University of California, San Diego* | **Michael Fogler**, *University of California, San Diego* | **Matt Zhang**, *University of California, San Diego* | **Zhao Hao**, *Lawrence Berkeley National Lab* | **Michael Martin**, *Lawrence Berkeley National Lab* | **Erik Henriksen**, *Columbia University, USA* | **Zhigang Jiang**, *Columbia University, USA* | **Philip Kim**, *Columbia University, USA* | **Horst Stormer**, *Columbia University, USA* | **Larry Carr**, *Brookhaven National Lab* | **Jie Shan**, *Case Western Reserve University* | **Chun Hung Lui**, *Columbia University, USA* | **Kin-Fai Mak**, *Columbia University, USA* | **Tony Heinz**, *Columbia University, USA*

I will present our recent investigations on graphene and multilayer graphene employing infrared spectroscopy. Our studies directly demonstrated the Dirac nature of the charge carriers in graphene from measurements of the Fermi energy, and revealed several signatures of many body interactions including excessive conductivity and Fermi velocity enhancement at low energy. In multilayer graphene, we found that the optical phonons (G mode) exhibit various unusual lineshapes characteristic of Fano resonances, which depend critically on the layer thickness and stacking order of the sample. We show that these observations can be understood in terms of the coupling between phonons and interband electronic transitions.

## 16:40-17:20 Invited Speaker

### Resonant and coherent Raman scattering in graphene

**Leandro Malard**, *Columbia University, USA; Universidade Federal de Minas Gerais, Brasil* | **Daniela Mafra**, *Universidade Federal de Minas Gerais, Brasil* | **H. Htoon**, *Los Alamos National Laboratory, USA* | **S. Doorn**, *Los Alamos National Laboratory, USA* | **A. H. Castro Neto**, *Boston University, USA* | **M. A. Pimenta**, *Universidade Federal de Minas Gerais, Brasil* | **Davide Boschetto**, *Columbia University, USA* | **Zhiqiang Li**, *Columbia University, USA* | **Chun Hung Lui**, *Columbia University, USA* | **Kin Fai Mak**, *Columbia University, USA* | **Tony Heinz**, *Columbia University, USA*

Raman spectroscopy has been playing an important role in unraveling the properties in graphene systems like disorder, doping and strain. Moreover the use of resonance Raman scattering in graphene has been shown to provide important information about the electronic and phonon dispersion in mono and bilayer graphene. For bilayer graphene by measuring the dispersion of the G' (2D) band for laser energies from the visible to the near infrared region we were able to probe the phonon dispersion close to the K point. Our data indicates a strong Kohn anomaly and that electron-electron interaction is important for describing the dispersion of optical phonons near the K point of graphene. We also studied the behavior of the Kohn anomaly in bilayer graphene near the zone center by changing charge carrier concentration with bottom and top gate voltages. Our results show that phonons in bilayer graphene are strongly mixed and have different behavior as a function of charge concentration. These results are well explained by the non-adiabatic Kohn anomaly in bilayer graphene by considering inhomogeneous charge carriers between the top and bottom layers. On a different approach to static Raman, we also perform measurements of the time dependent reflectivity of graphene layers in a pump-probe experimental scheme. We could observe the time dependent evolution of the shearing phonon mode as a function of number of graphene layers. Our result shows a strong stacking dependence which allows the investigation of intrinsic phonon properties evolution from bidimensional to bulk in graphene systems.

## Posters

### Graphene on the 6H-SiC(000-1)(3x3) surface reconstruction: an almost ideal graphene layer?

**Fanny Hiebel**, *Institut Neel CNRS-UJF* | **Pierre Mallet**, *Institut Neel CNRS-UJF* | **Laurence Magaud**, *Institut Neel CNRS-UJF* | **Jean-Yves Veuillen**, *Institut Neel CNRS-UJF*

Since the experimental discovery of the exceptional electronic properties of graphene, enthusiasm has kept growing. In-depth investigations of the material or industrial uses require high quality samples. In particular, the influence of the environment is an important issue. Hence, well reproducible substrates, showing minimal interaction with the graphene layer are desirable. We have grown graphene on the 6H-SiC(000-1) surface, by thermal desorption of Si under ultra-high vacuum. In situ characterization was performed at room temperature by scanning tunneling microscopy and spectroscopy. The samples present monolayer graphene islands on two types of interfaces, identified as native surface reconstructions. We concentrate here on the graphene on SiC(000-1)(3x3) system (Hiebel et al., Phys. Rev. B 80, 235429 (2009)). Taking advantage of the transparency of graphene in high bias voltage images, we first show that the superstructures of various periodicities observed on the islands are moiré patterns. We then identify the corresponding graphene - substrate stacking. A study of the moiré corrugation versus sample bias voltage suggests a topographic corrugation of the graphene layer, arising from a very small stacking-dependent interaction with the substrate. Indeed, spectroscopic imaging shows that the electronic structure of the graphene layer is spatially homogeneous. Finally, the bare (3x3) surface exhibits a wide surface gap that subsists under the graphene layer, suggesting a very small coupling in this energy range. We conclude that graphene on (3x3) is nearly ideal for investigating low energy excitations of the system.

### Band gap engineering of graphene by strain

**Seung-Hoon Jhi**, *Pohang University Of Science And Technology* | **Seon-Myeong Choi**, *Pohang University Of Science And Technology* | **Young-Woo Son**, *Korea Institute for Advanced Study*

Mechanical strain often gives rise to surprising effects on electronic properties of carbon nanomaterials. The influence of smooth elastic deformations on the physics of graphene can be described by introducing a suitable gauge-field vector potential to the free massless particle Dirac¡¯s equation. Here we present first-principles calculations of electronic properties of single and bilayer graphene under strain. For single layer graphene, the semi-metallic nature is shown to persist up to a very large uniaxial strain of 30% except a very narrow strain range where a tiny energy gap opens. In very high strain regime, the sigma-band shifts down to close the gap. The low energy properties with small uniaxial strains can be described by the generalized Weyl¡¯s equation while massless and massive electrons coexist with large ones. The work function is also predicted to increase substantially as both the uniaxial and isotropic strain increases. For bilayer graphene, we show that mechanically tunable electronic energy gap is realizable if different homogeneous strains are applied to the two layers. It is shown that the size of energy gap can be simply controlled by adjusting the strength and direction of these strains. If homogeneous strains with different strengths are applied to each layer of bilayer graphene, transverse electric fields across the two layers can be generated without any external electronic sources, thereby opening an energy gap. The results demonstrate a simple mechanical method of realizing pseudo-electromagnetism in graphene and suggest a maneuverable approach to fabrication of electromechanical devices based on bilayer graphene.

### Strain-tunable suspended graphene quantum dots

**Vahid Tayari**, *Concordia University, Department of Physics,Canada* | **Joshua Island**, *Concordia University, Department of Physics, Canada* | **Alexandre Champagne**, *Concordia University, Department of Physics, Canada*

We are fabricating 10-nm scale suspended graphene quantum dots (QDs), and will study electron-vibron coupling in these structures as a function of strain, charge density and temperature. We make use of a specialized experimental method called gated-mechanical break-junction (g-MCBJ) which can simultaneously tune the mechanical strain applied to our nm-sized graphene QDs and their electron density. The g-MCBJ technique controls the spacing between the source and drain electrodes of the QDs with picometer resolution by bending the substrate above which the electrodes are suspended. The substrate we use is doped silicon and acts as a gate electrode to tune the charge carrier density in the QDs. By tuning the strain in our QDs, we aim to control their vibronic spectrums, the strength of their electron-vibron couplings, and develop extremely sensitive NEMS sensors. We present the fabrication of our devices, the g-MCBJ apparatus, and initial electron transport data in our strain tunable QDs.

### Measurements of Heat Transport in Graphene

**Serap Yigen**, *Concordia University, Department of Physics, Canada* | **Maryam Tabatabaei**, *Concordia University, Department of Physics, Canada* | **Alexandre Champagne**, *Concordia University, Department of Physics, Canada*

We present our progress towards measuring heat transport in micron-scale suspended graphene samples to assess graphene’s promising potential for thermal management in nanoscale electronics, and test the theoretical models of heat propagation in graphene. Heat is carried by both electrons and phonons, and measuring heat transport in graphene is a powerful tool to obtain information about its phonon modes, electronic band structure, and electron-phonon interactions. We are fabricating suspended graphene devices on which we place nanowires which act as heater and thermometers. We will use joule heating in one nanowire to drive the heat current and use a second wire as a thermometer to measure heat conductivity. The absence of heat leakage to the substrate (suspended device) will allow a quantitative measurement of heat conductivity. Using the gate electrode placed under our graphene crystal we will make direct measurements of heat conductivity versus electron density, temperature and magnetic field. We present the fabrication of our devices, and preliminary electron and heat transport data from our samples.

### Spin-Unrestricted Calculations of Bare-Edged Nanographenes Using DFT and Many-Body Perturbation Theory

**Hakim Amara,** *Laboratoire d’Etude des Microstructres, Onera-Cnrs, France* | **Rodolphe Pollet**, *Laboratoire Claude Fréjacques, CEA, France*

The ability of Density Functional Theory to predict the electronic and magnetic properties of semiinfinite graphene with a single bare edge has been probed. In order to improve the accuracy of spin-unrestricted calculations performed with semilocal density functionals, higher-level methods including double hybrid density functionals and many-body perturbation theory have been applied to the polycyclic aromatic hydrocarbons model systems. We show that the antiferromagnetic or ferromagnetic tendencies of the corresponding electronic ground states strongly depend on the choice of the density functional. In addition the relative stability of the armchair and zigzag edges has been investigated, emphasizing the importance of using methods beyond semilocals density functionals [1]. [1] R. Pollet and H. Amara, J. Chem. Theory Comput. 5 1719 (2009)

### Dynamic superlubricity of graphene flake on graphite surface

**Irina Lebedeva**, *Moscow Institute of Physics and Technology, Russia; RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Moscow, Russia* | **Andrey Knizhnik**, *RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Moscow, Russia* | **Andrey Popov**, *Institute of Spectroscopy, Russia* | **Olga Ershova**, *Moscow Institute of Physics and Technology, Russia* | **Yurii Lozovik**, *Institute of Spectroscopy, Russia* | **Boris Potapkin**, *RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Moscow, Russia*

Different mechanisms of diffusion and drift of a graphene flake on a graphite surface are systematically analyzed using ab initio calculations and calculations with empirical potentials. A new mechanism of diffusion, “dynamic superlubricity”, is proposed. According to the proposed mechanism, rotational transition of the flake to incommensurate states takes place with subsequent simultaneous rotation and translational motion until the commensurate state is reached again, and so on. Due to the significant barrier for rotation of the flake, these events are rare. However, this factor is compensated by long distances passed by the flake before it returns to the commensurate state. The molecular dynamics simulations demonstrate that the proposed diffusion mechanism can be dominant under certain conditions. According to analytic expressions derived for the diffusion coefficient and mobility of the flake, the relative contribution of rotation to incommensurate states should be the most significant at temperature associated with the barrier for transition of the flake between adjacent energy minima in the commensurate state and should correspond to an increase of the diffusion coefficient by more than an order of magnitude. The results obtained can be also useful for study of dynamics of polyaromatic molecules on a graphite surface and should be qualitatively valid for a set of commensurate adsorbate-adsorbent systems. The methods of control over the diffusion and drift of graphene components in nanoelectromechanical systems are discussed. Moreover, the possibility to experimentally measure the barriers to relative motion of graphene layers by study of a graphene flake diffusion is considered.

### Molecular dynamics and kinetic modeling of phonon transport in defective carbon nanostructures

**Andrey Knizhnik**, *Kintech Lab Ltd., Moscow, Russia* | **Inna Iskandarova**, *Kintech Lab Ltd., Moscow, Russia* | **Dmitry Krasikov**, *Kintech Lab Ltd., Moscow, Russia* | **Alexander Eletskii**, *Kintech Lab Ltd., Moscow, Russia* | **Boris Potapkin**, *Kintech Lab Ltd., Moscow, Russia* | **Vinayak Tilak**, *GE Global Research, Niskayuna, New York, USA* | **Kamala Raghavan**, *GE Global Research, Bangalore, India*

Low dimensional carbon nanostructures, such as carbon nanotubes, graphene, possess unique physical properties, in particular, high thermal conductivity. These unique physical properties depend strongly on the structural and compositional characteristics of nanostructures. Atomistic methods, such as equilibrium and non-equilibrium molecular dynamics, are widely used to investigate dependence of thermal conductivity on the structure of the nanomaterial, in particular on the number and nature of defects. However, atomistic methods have severe drawbacks in considering real nanostructures due to the spatial and temporal limitation. At the same time, available macroscopic methods, such as kinetic Boltzmann equation, can overcome size limitations of atomistic methods, but cannot predict accurately scattering properties of structural and compositional defects. In this work we present the results of combination of molecular dynamics method for calculation of thermal conductivity with macroscopic method based on Boltzmann transport equation. We made direct comparison of these two methods using parameters of macroscopic model derived from the results of atomistic simulations of intermediate-size systems. We also performed investigation of influence of point defects on thermal transport in graphene using molecular dynamics and Boltzmann transport equation model. While systems with super micron-scale cannot be considered now directly with molecular dynamics methods, we were able to describe thermal properties of these systems using combined approach. Based on the results of the proposed approach we investigate the effect of different types of defects on thermal conductivity and determine the critical fraction of point defects in the carbon nanostructures as a function of their length.

## High energy magneto-optical spectroscopy of epitaxial graphene and graphite

**Nicolas Ubrig**, *Laboratoire Nationale Des Champs Magnétiques Intenses* | **Paulina Plochocka**, *Laboratoire Nationale Des Champs Magnétiques Intenses* | **Piotr Kossaki**, *Laboratoire Nationale Des Champs Magnétiques Intenses; Institute of Experimental Physics, University of Warsaw, Poland* |**Marek Potemski**, *Laboratoire Nationale Des Champs Magnétiques Intenses* |**Oliver Portugall**, *Laboratoire Nationale Des Champs Magnétiques Intenses*

The discovery of massless relativistic particles in graphene, a monolayer of graphite, has completely renewed the interest in graphite and his allotropes. This spectacular new discoveries propulsed graphene as one of the most promising material with application potential in electronics. The epitaxial growth of graphene on a SiC substrate opened the door to optical spectroscopy on graphene where the scenario of massless dirac fermions with a square root B landau level dependence could be confirmed by FIR transmission measurements[1]. In order to get a deeper understanding of the bandstructures of graphene and graphite we investigate this materials in the high-energy limit at very high magnetic fields. For graphene the linear approximation is not valid anymore in this region under the influence of trigonal warping. This effect can be written in the equations of bandstructure of graphene and give rise to an asymmetry in the landau level transitions between hole-electron and electron-hole. With the help of polarisation resolved magneto-optical spectroscopy in fields up to 60 Tesla we are able to detect the predicted asymmetry. Trigonal warping terms are found in the description of the bandstructure of graphite too, according to the theory of Slonczewski, Weiss and McClure. A comprehensive comparison is made between the spectra of graphite and graphene in the same energy region up to 60 Tesla and for different temperatures in order to compare the influence of trigonal warping which is present in both materials. [1] M.Sadowski et al., PRL 97 (2006)

## Visibility of graphene monolayers on various substrates

**Victor Yu**, *McGill University* | **Michael Hilke**, *McGill University*

The structure of the substrate played a significant role in the observation of graphene monolayers [1]. In particular, the oxide layer thickness is crucial in order to identify graphene monolayers by optical contrast. Here we consider new ways to increase this optical contrast in order to allow the identification of monolayers on various substrates. We studied the contrast enhancement obtained by tilting the sample with respect to the optical incidence [2]. For SiO2/Si substrates, with an oxide thickness of 90nm we obtained an enhanced contrast of up to 50% when using a polarizer and a filter at an incident angle of 65 degrees. This should be compared to a maximum contrast of 15% when the light is normally incident. We also showed experimentally that graphene can be observed on GaAs/AlGaAs heterostructures, where we obtain an optical contrast of about 12% by tilting the sample to 65 degrees. The situation of graphene on copper will also be discussed. [1] P. Blake, K. S. Novoselov, A. H. Castro Neto, D. Jiang, R. Yang, T. J. Booth, A. K. Geim, and E. W. Hill, Appl. Phys. Lett. 91 063124 (2007). [2] V. Yu and M. Hilke, Appl. Phys. Lett. 95 151904 (2009).

## Binary transmission through selectively biased, doped,or variable-width graphene nanoribbons

**Elham Rezasoltani**, *Physics Department Concordia University* | **Panagiotis Vasilopoulos**

We present results for the electronic transmission through single and double barriers in single-layer armchair and zigzag graphene nanoribbons. We selectively consider barriers that result either from the application of gates (potential barriers) or from the modulation of the Fermi velocity vF (velocity barriers) and compare the results,when possible, with those obtained from tight-binding treatments. The transmission is qualitatively similar for both kinds of barriers, vanishes for zero angle of incidence,shows resonances at certain angles similar to those in unconfined graphene [1], and is affected by the discreteness of the wave vectors due to the confinement along the ribbon width. Further, we investigate graphene nanoribbons of piecewise constant width (stubbed nanoribbons) and show that the transmission, as a function of the stub length and/or width, exhibits a square-wave behavior appropriate to transistors. 1. M. I. Katsnelson et al., Nature Phys. 2, 620 (2006); J. M. Pereira Jr. et al., Phys. Rev. B 74, 045424 (2006).

## Surface potential and charge distribution in graphene: An Electrostatic Force Microscopy study

**Ather Mahmood**, *Institut NEEL, CNRS, France* | **Thierry Mélin**, *Institute for Electronics, Microelectronics and Nanotechnology (IEMN-CNRS), France* | **Dominique Vuillaume**, *Institute for Electronics, Microelectronics and Nanotechnology (IEMN-CNRS), France* | **Erik Dujardin**, *Centre d'Elaboration de Matériaux et d'Etudes Structurales (CEMES-CNRS), France*

Electrostatic Force Microscopy (EFM) [Martin Y et. al. App. Phys . Lett. 52, 1103, (1998)] is able to distinguish electric forces resulting from charge distribution in nanostructures from the capacitive interaction [T. Heim, et.al. NanoLett. 4, 2145-2150 (2004)]. Some of the intrinsic electrical properties can readily be determined in a non-destructive manner, and without the need of electrical contacts. We present the application of EFM to probe the surface potential and charge spread in single and few layered exfoliated graphene sheets and ribbons deposited on Si wafers. The wide expanse of graphene sheets make it reasonable to treat graphene like an anisotropic dielectric layer where infinite and finite values of in-plane and transverse dielectric constant, respectively, renders graphene as an in-plane metal. Experimental results are shown to correspond with simulations, based on solving Poisson's equations, to deduce the force gradients on the tip as a function of the graphene-tip distance. Further, the metallic tip is used to establish contact and inject charge in garphene layers, in order to probe the 2-D charge spread as a function of number of layers. Finally, the same approach is applied to the static characterization of the graphene nanoribbons fabricated within a double side-gated device on mono- and few-layered graphene sheets, using Focused Ion Beam (FIB) irradiation.

## A multi-scale approach for the performance assessment of hydrogenated graphane Field-Effect Transistors

**Gianluca Fiori**, *Information Engineering Department, University Of Pisa* | **Sebastien Lebègue**, *Institut Jean Barriol, Nancy Université* | **Alessandro Betti**, *Information Engineering Department, University Of Pisa* | **Paolo Michetti**, *Theoretical Physics and Astrophysics, University of Wuerzburg* |**Mattias Klintenberg**, *Department of Physics and Astronomy, Uppsala University* |**Olle Eriksson**, *Department of Physics and Astronomy, Uppsala University* |**Giuseppe Iannaccone**, *Information Engineering Department, University Of Pisa*

In this work, we present, for the first time, the performance analysis of Field Effect Transistors based on recently fabricated 100% hydrogenated graphene [1] (the so-called graphane) and theoretically predicted semi-hydrogenated graphene (i.e. graphone) [2]. The multi-scale approach is based on accurate calculations of the energy bands by means of GW approximation, subsequently fitted with a three-nearest neighbour (3NN) sp3 tight-binding Hamiltonian, and finally used to compute semiclassical transport in transistors based on functionalized graphene. In particular, the GW calculations have provided accurate values for the energy bands and band-gaps, which, in the case of graphone, has been demonstrated to differ by more than 2.7 eV from recently obtained results through DFT-GGA [2]. Transport results have shown that graphane and graphone based FETs can provide large current as well as Ion/Ioff ratios, and can represent a promising option for future technology nodes. Indeed, due to the large energy gap, the proposed devices have many of the advantages provided by one-dimensional graphene nanoribbon FETs, such as large Ion and Ion/Ioff ratios, reduced band-to-band tunneling, without the corresponding disadvantages in terms of prohibitive lithography and patterning requirements for circuit integration. References [1] D. Elias et al. Science 2009, 323, 610 [2] J. Zhou et a.l Nano Lett. 2009, 9, 3867

## Probing coupled electronic and vibrational states in Graphene Oxide using fluorescence spectroscopy

**Charudatta Galande**, *Department of Mechanical Engineering and Materials Science, Rice University, USA* | **Aditya Mohite**, *Center for Integrated Nanotechnologies, Los Alamos National Laboratory, USA* | **Anton Naumov**, *Applied Physics Program, Rice University, USA* | **Wei Gao**, *Department of Chemistry, Rice University* | **Hui Gao**, *Department of Mechanical Engineering and Materials Science, Rice University, USA* | **Anchal Srivastava**, *Department of Physics, Banaras Hindu University, India* | **R.Bruce Weisman**, *Department of Chemistry, Rice University* | **Pulickel M. Ajayan**, *Department of Mechanical Engineering and Materials Science, Rice University, USA; Department of Chemistry, Rice University*

Graphene Oxide (GO) is a functionalized derivative of graphene, obtained by chemical exfoliation and chemical oxidation of graphite. Recent NMR studies on GO have revealed presence of several functional groups - mainly hydroxyl, epoxy, carbonyl, carboxyl and lactols. Although there have been several studies on electronic and optical properties of GO, the role of functional groups in determining the electronic density of states is still unclear. Here we report pH-dependent fluorescence and excitation spectra of GO, with spectroscopic signatures indicating coupling of electronic transitions and vibrational modes of functional groups. At pH 1.7, a single, broad (~200 nm FWHM) fluorescence peak is observed near 660nm. Tuning the sample pH from acidic to basic results in complete quenching of this peak by pH 11. In addition, new emission features at lower wavelengths (480 nm - 515 nm) appear in a narrow pH range between 7.8 and 8.0 and completely dominate the spectrum by pH 11. In this basic environment, the excitation and emission spectra show several similar features in a mirror image pattern such as those seen in molecular spectroscopy. These suggest significant vibrational-electronic coupling related to the functional groups. Understanding how functional groups influence the optical properties of GO may enable controlled manipulation of the Graphene electronic band structure.

## Imaging Potassium atoms on the surface of HOPG graphite by STM

**Julien Renard**, *Department of Physics and Astronomy, University Of British Columbia* | **Yan Pennec**, *Department of Physics and Astronomy, University Of British Columbia* | **Mark Lundeberg**, *Department of Physics and Astronomy, University Of British Columbia* **Joshua Folk**, *Department of Physics and Astronomy, University Of British Columbia* | **Doug Bonn**, *Department of Physics and Astronomy, University Of British Columbia*

The interaction of alkali atoms with graphitic surfaces has been extensively studied in the past twenty years. One reason for this interest is the possibility to dramatically modify the electronic structure of graphite with alkali intercalation[1], leading to superconductivity in some cases. Besides the modification of the electronic properties, the adsorption of alkali onto graphitic surfaces presents a very rich structural phase diagram[2]. Although many studies were performed, including structural and spectroscopic studies, no evidence of these structural phases by local probe techniques were reported so far. We report the observation by STM of the diluted phase of potassium atoms adsorbed on HOPG graphite. The study was performed at low temperature(10K) under ultra high vacuum conditions(~10-10mbar). At coverages in the range of 0.01 monolayer, we successfully observe single potassium atoms separated by distances of several nanometers. This is a consequence of their electrostatic repulsion resulting from the efficient charge transfer to the graphite[2,3]. We will discuss the structure of this diluted potassium phase. Even at 10K, a slow diffusion of the potassium on the surface could be monitored by recording successive STM images. Based on the diffusion rate of the potassium atoms, we can estimate the diffusion barrier and compare our estimations with recent calculations made by density functional theory[4]. [1] T. Enoki et al, Graphite Intecalation Compounds and Applications, Oxford University Press (2003) [2] Mellita Caragiu et al, J.Phys.Condens.Matter 17, R995(2005) [3] Z. Y. Li et al Phys.Rev.Lett. 67 1562(1991) [4] K. Rytkönen et al Phys.Rev.B 75 075401(2007)

## Photo-Chemical Reduction of Graphene Oxide by Ultraviolet Laser Lithography

**Peter Gaskell**, *McGill University, Canada* | **Helgi Skulason**, *McGill University, Canada* | **Tarun Chari**, *McGill University, Canada* | **Mohamed Siaj**, *Université de Québec à Montréal* | **Thomas Szkopek**, *McGill University, Canada*

We report the reduction of graphene oxide into graphene via exposure to UV light, with evidence for a photo-chemical process. Graphene oxide samples are prepared by modified Hummer's method from bulk graphite and deposited on sodalime glass and oxidized silicon substrates. Graphene oxide is reduced using a 15mW 370nm diode laser focused to a 5um spot. Monitoring the change in reflected light during photo-reduction allows an in situ measure of the level of reduction. The rate of reduction is dependant on the intensity of light on the sample. No change in reflectance is observed when illuminating samples with a 632nm HeNe laser at similar intensities and exposure times providing evidence of a photochemical effect  Raman spectra taken at varying levels of reduction show a clear enhancement of the G and D bands, approaching that of graphene oxide reduced chemically with hydrazine vapor. Ellipsometry and optical reflection contrast measurements and electrical conductance measurements of UV reduced graphene oxide will also be presented. Direct write UV lithographic exposure and edge diffraction were used to define reduced graphene oxide stripes with 5um and 2um pitch respectively. Formed with long exposure times greater than 10 minutes, we hypothesize that the 2um pitch gratings are inconsistent with thermal reduction owing to the large thermal gradients that would ensue. UV reduction of graphene oxide could provide a simple resist-free method of patterning conductive circuits into an insulating material and is compatible with current UV lithography technologies used in semiconductor manufacturing.

## Large-Area CVD Growth of Graphene for electronic and energy conversion applications

**Chongwu Zhou**, University Of Southern California

The advance of graphene-based electronics has been hampered due to the difficulty in producing single or few-layers graphene over large areas. We will present the synthesis of graphene using chemical vapor deposition (CVD) over wafer scale [1] and macroscopic area, and report the application of CVD graphene for transistors and transparent conductive electrodes for organic photovoltaic devices [2]. Systematic study has performed to compare the synthesis on polycrystal Ni film, single crystal Ni (111), and copper foil. We observed the preferential formation of single- and bilayer graphene over ~90% of the single crystal surface of Ni (111). In addition, we achieved the first implementation of continuous, highly flexible, and transparent CVD graphene films as transparent conductive electrodes (TCE) in organic photovoltaic cells. Graphene films were synthesized by chemical vapor deposition, transferred to transparent substrates, and evaluated in organic solar cell heterojunctions. Solar cells with CVD graphene and ITO electrodes were fabricated on flexible polyethylene terephthalate (PET) substrates, and confirmed to offer as good performance, with power conversion efficiencies of 1.18 and 1.27 %, respectively [2]. Our work indicates the great potential of CVD graphene films for macroscopic scale processing of graphene-based electronics and flexible transparent electronics. [1]. "Synthesis, Transfer, and Devices of Single- and Few-Layer Graphene by Chemical Vapor Deposition" Chongwu Zhou et al., IEEE Transactions on Nanotechnology, Vol. 8, pp. 135, 2009. [2]. "Continuous, Highly Flexible, and Transparent Graphene Films by Chemical Vapor Deposition for Organic Photovoltaics" Chongwu Zhou et al., ACS Nano, 2010 (accepted).

### Graphene-on-Au(111): a Highly Conductive Material with Excellent Ability of the Adsorption for High-resolution Bio-/Nano-detection and Identification

**Bo Song**, *Shanghai Institute Of Applied Physics, Chinese Academy Of Sciences* | **Di Li** | **Wenpeng Qi** | **Marcus Elstner** | **Chunhai Fan** | **Haiping Fang**

Based on numerical simulations and experimental studies, we show that, a composition of a sheet of graphene on a Au(111) surface exhibits both the excellent conductivity and the ability to stably adsorb the biomolecules. If we use it as a substrate, the signal-to-noise ratios can be greatly enhanced. The key to this unique property lies in the graphene can stably adsorb carbon-based rings widely existing in biomolecules due to ¦Ð-stacking interactions, while the substrate retains excellent conductivity from metallicity of the gold. Remarkably, the signal-to-noise ratio is found to be so high that the signal is clearly distinguishable for different nucleobases when an ssDNA is placed on this graphene-on-Au(111). Our finding opens opportunities for a range of bio-/nano- applications including single-DNA-molecule-based bio-devices and biosensors, particularly high-accuracy sequencing of DNA strands with repeating segments.

### Surfactant stabilised graphene dispersions at high concentration

**Mustafa Lotya**, *School of Physics, Trinity College Dublin, Ireland; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland* | **Paul King**, *School of Physics, Trinity College Dublin, Ireland; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland* | **Umar Khan**, *School of Physics, Trinity College Dublin, Ireland; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland* |**Sukante De**, *School of Physics, Trinity College Dublin, Ireland; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland* | **Jonathan Coleman**, *School of Physics, Trinity College Dublin, Ireland; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland*

Graphene has generated intense research interest in recent years due to its unique physical properties. Our group has concentrated on producing liquid-phase dispersions of pristine graphene to facilitate materials processing and the development of graphene thin films. This submission focuses on the stable suspension of graphene at high concentration in aqueous media with the aid of the surfactant sodium cholate. This study compliments earlier work done by our team and others on surfactant-stabilised graphene. We show that under mild sonication for long times, graphene concentrations up to 0.3 mg/ml are attainable using just 0.1 mg/ml of surfactant. We studied the effect of centrifugation speed on the dispersions finding an empirical scaling of graphene concentration. We also used Raman spectroscopy and TEM analysis to assess the graphene quality and level of exfoliation. Finally, we show that high quality free-standing graphene films can be easily fabricated by our solution processing methods.

### Quantitative & Qualitative Analysis of Various Surfactant-Exfoliated Graphene Dispersions

**Ronan Smith**, *School Of Physics, Trinity College Dublin; CRANN, Trinity College Dublin* | **Mustafa Lotya**, *School Of Physics, Trinity College Dublin; CRANN, Trinity College Dublin* | **Paul King**, *School Of Physics, Trinity College Dublin; CRANN, Trinity College Dublin* | **Jonathan Coleman**, *School Of Physics, Trinity College Dublin; CRANN, Trinity College Dublin*

Recent work has shown a method to disperse and exfoliate graphite to give graphene suspended in water-surfactant solutions[1,2] This process has many advantages over solvent based exfoliation[3] including bio-compatibility, safe processing and low cost. Very few surfactants have been tested for this process and very little work has been done to compare different types of surfactant with a view to optimization of dispersion yield and quality. In this work, graphite has been exfoliated to give graphene using various anionic, cationic and non-ionic surfactants. 12 surfactants are compared based on their exfoliation efficiency at a fixed low surfactant concentration. The dispersion yields are compared using absorption spectroscopy while dispersion quality is assessed using TEM and Raman Spectroscopy. References [1] Lotya et al. Journal of the American Chemical Society 2009, 131, 3611. [2] Green et al. Nano letters 2009, 9 (12), 4031. [3] Hernandez et al. Nature Nanotechnology 2008, 3, 563.

## 18:00-20:00 NT10 Welcome Reception

# TUTORIALS

## ROOM: VERDUN

## Monday, June 28

### 13:00-14:00 Tutorial A

**Nucleation and Growth of Carbon Nanotubes**

**David Geohegan**, *Center for Nanophase Materials Sciences and Materials Science and Technology Division, Oak Ridge National Laboratory* | **Alex Puretzky**, *Center for Nanophase Materials Sciences and Materials Science and Technology Division, Oak Ridge National Laboratory* | **Gyula Eres**, *Center for Nanophase Materials Sciences and Materials Science and Technology Division, Oak Ridge National Laboratory* | **Chris Rouleau**, *Center for Nanophase Materials Sciences and Materials Science and Technology Division, Oak Ridge National Laboratory*

The desire to understand the nucleation and growth mechanisms of carbon nanotubes is driven partly by fundamental scientific curiosity, but also by the need to control their properties for specific applications. This is especially true for single-walled carbon nanotubes, where efforts continue to control their precise atomic structure through controlled synthesis are the key to many applications. This tutorial will cover the fundamental principles of carbon nanotube synthesis through a review of experimental nanotube growth methods , associated in situ diagnostic experiments and techniques, practical growth models, and atomistic theoretical simulations of nucleation and continued growth. The tutorial traces the development of both theoretical and experimental understanding of nanotube nucleation and growth mechanisms through a historical review of key developments in experimental synthesis techniques and associated in situ diagnostics of nanotube growth. Advances in the understanding of the mechanisms by which nanotubes nucleate and grow, including both high- and low-temperature growth environments, are reviewed through exciting experimental discoveries which revealed clues to the synthesis process. The review will end with present challenges and recent developments. Supported by U.S. Dept. of Energy, Basic Energy Sciences, Division of Materials Science and Engineering.

### 14:00-15:00 Tutorial B

**Nanotube structure determination and population evaluation with Transmission Electron Microscopy and Spectroscopies**

**Annick Loiseau**, *LEM, Onera-Cnrs, France*

This tutorial will introduce the fundamentals of the structure characterization of nanotubes and discuss its current status, with a particular attention paid to the study of individual tubes compared to the population evaluation of a macroscopic sample. First part will focus on Transmission Electron Microscopy (TEM) capabilities. TEM has been shown to be an essential tool for determining the nanotube structure. Different modes – electron diffraction, high resolution imaging, electron energy loss spectroscopy – can provide direct quantitative information on diameter, number of layers, helicity, chemical composition and chemical environment of a given tube. The talk will discuss how to use TEM tools for evaluating a population of tubes by achieving statistical analyses. Second part will cross-check TEM data with spectroscopic measurements. These tools are also widely used for structural characterization, as they are capable of easily inspecting macroscopic samples. However, in these techniques, structure parameters are extracted only via a relationship between the atomic structure and a measured given property (vibrational, electronic, optical…). The difficulty crucially lies in the knowledge of the link structure-property and of the tube environment in the sample. In the recent years, progress made in the techniques and in the sample manipulation has made possible the study of individual tubes, opening the way to multiple diagnostics on a given tube and to a direct comparison with TEM data. The talk will discuss the impact of the advances for both the knowledge of the tube structure and the improvement of the characterization techniques.

### 15:00-15:30 Coffee Break

### 15:30-16:30 Tutorial C

**Fundamentals of the optical properties of carbon nanotubes and current status**

**Anna Swan**, *Boston University*

Optical spectroscopy is of great use in order to reveal a materials' physical properties, such as its electronic structure, the vibrational properties, and their interactions and excited state de-excitation dynamics. In recent years we have experienced tremendous advancement in the understanding of optical properties of carbon nanotubes. Single wall carbon nanotubes come in a variety of different chirality, and the electronic properties are determined by the tube chirality given by the chiral vector, denoted (n,m). The one-dimensional structure gives rise to singularities in the electronic density of states, and strong Coulomb interactions that gives rise to strongly bound excitons from optical excitations. The strong resonance structure has enabled Raman spectroscopy on the single tube level, but despite this promising structure, it took over a decade from their initial discovery in 1991 to observe photoluminescence from carbon nanotubes, and it has been hard to determine such basic optical properties as optical crossection, intrinsic quantum efficiency, and radiative lifetime. I will discuss some historical perspective of the advancement of the field using spectroscopic methods (Raman scattering, Rayleigh scattering and Photoluminescence excitation spectroscopy), the current status and implications for applications.

### 16:30-17:30 Tutorial D

**Graphene and Carbon Nanotubes Electronics and Optoelectronics**

**Phaedon Avouris**, *IBM T. J. Watson Research Center, USA*

Nanoscience/nanotechnology is currently one of the most active areas of scientific research. At the nanometer scale, and in reduced dimensionality, materials acquire novel properties. This motivates the synthesis, manipulation, study and search for new applications of nanostructures. Among these, carbon-based nanostructures, carbon nanotubes and graphene, are attracting special attention. These single atom thick, low dimensional materials have some rather unique electrical and optical properties that recommend them for a host of different applications in electronics and photonics. In this talk we will discuss their electronic structure, their electronic and photonic properties, and demonstrate model electronic devices such as ultra-fast transistors, simple integrated circuits, optical detectors, infrared light emitters and saturable absorbers. We will discuss the physical basis of these devices, their advantages and also the hurdles that remain before they can be integrated into mature, competitive technologies.

### 18:00-20:00 NT10 Welcome Reception

# Main Conference Program

## ROOM: MONTREAL BALLROOM

## Tuesday, June 29

### 8:20 Opening Remarks

**SESSION CHAIR: MORINOBU ENDO,** *Shinshu University*

### 8:30-9:10 Keynote 1

**The Diverse and Growing Family of Carbon Nanotube and Related Artificial Muscles**
**Ray Baughman**, *The University Of Texas At Dallas, USA*

Collaborative work with colleagues at the University of Texas at Dallas, the University of Wollongong, the University of British Columbia, and Hanyang University has expanded the family of carbon nanotube artificial muscles from our original double-layer driven tensile muscles to pneumatic muscles, fuel driven muscles, giant stroke aerogel muscles, and even muscles that provide torsional actuation. These muscles, as well as carbon nanotubes muscles demonstrated by others, are here described. Extreme performance is demonstrated, like for our aerogel muscles that generate giant strokes and stroke rates of 220% and 3.7 x 104 %/s, respectively, from near 0 K to over 1900 K; electrochemical muscles that generate a hundred times the tensile stress of natural muscle; and torsional muscles that rotate at up to 600 revolutions per minute and provide a hundred times higher rotation per unit length than previous torsional muscles. The properties of these electrically powered muscles, and related fuel powered muscles, are described and theoretically explained.

### 9:10-9:27 Contributed Talk 1

**Compounding and processing of PA 6/MWCNT Composites**
**Cecile Gibon**, *BASF SE, Germany* | **Christof Kujat** | **Xin Yang** | **Christof Wigbers** | **Hennig Ingolf** | **Steininger Helmut** | **Weber Martin**

The transfer of Carbon Nanotube properties to macroscopic materials is still a non-solved issue. The development of adapted processing methods is therefore a compulsory step for the improvement of the compound performances. To that purpose, BASF SE has started research activities to develop dispersion technologies for CNTs in different matrices (thermoplastics or thermoset systems). The presentation will review the work related to CNTs in thermoplastics, an example is given in PA6 matrix. First experiments focused on the compound and masterbatch preparation using the kneader technology. The investigations showed that this technology can be efficiently used for the dispersion of CNTs in PA6. The preparation of agglomerate-free masterbatches with loading contents of 15 wt.-% could be achieved. Nevertheless long residence times are needed to reach good dispersion states, leading to PA6 degradation. Furthermore compounds were prepared either through dilution of different masterbatches (commercial ones or prepared in the kneader) or through direct compounding. The processing occurs in an extrusion step followed by injection molding. The obtained products were characterized in terms of dispersion quality, electrical and mechanical properties. These properties are compared to those of benchmark materials such as carbon black. Percolation thresholds can be significantly reduced by the use of CNTs compared to other fillers, however this percolation strongly depends on the processing parameters. Under standard PA6 injection molding conditions, percolation concentrations are still too high to ensure sufficient mechanical properties of the compounds: processing conditions have to be tuned to reach the targeted properties.

### 9:27-9:44 Contributed Talk 2

**Novel boron nitride nanofillers for polymeric composites**
**Chunyi Zhi**, *National Institute For Materials Science, Japan* |
**Yoshio Bando**, *National Institute For Materials Science, Japan* |
**ChengchunTang**, *National Institute For Materials Science, Japan* |
**Golberg Dmitri**, *National Institute For Materials Science, Japan*

Boron nitride nanomaterials are valuable due to their constant wide band gap, high thermal conductivity, superb structural stability and chemical inertness. These characteristics make them primarily important for novel nanofillers in thermo-conductive and electrically insulating polymeric composites, or for functional units in electronic devices working in hazardous and/or high-temperature environments. According to many well-established models, nano-size materials with high aspect ratio can be much more effective fillers for property improvements of matrixes. Therefore, compared with conventional micro-size particles, BN nanostructures, such as nanotubes and nanosheets are very promising next-generation nanofillers for thermal conductivity improvement and mechanical reinforcement of matrix. We developed a special CVD method and realized grams level synthesis of BN nanotubes, which make it possible to initiate a study of their utilization in composites. Subsequently, BN nanotube containing polymeric composites were fabricated using several polymers as matrixes and their thermal, electrical and mechanical properties were evaluated. More than 20-fold thermal conductivity improvement in BN nanotube-containing polymers was obtained, and such composites keep good electrical insulation. The coefficient of thermal expansion (CTE) of BN nanotube loaded polymers was dramatically reduced due to the interactions between polymer chains and the nanotubes. The composites possess excellent functional performance, as revealed by systematic mechanical and dielectric property investigations. In addition, through adopting a liquid exfoliation method, milligrams level ultrathin BN nanosheets were fabricated. Characterizations of BN nanosheet-containing polymeric composites indicated that a 22% improvement of the elastic modulus of PMMA could be obtained with only 0.3 wt.% BN nanosheet loading fraction used.

### 9:44-10:01 Contributed Talk 3

**Non-Dispersive Built, Aligned SWNT Prepreg Sheet**
**Kazufumi Kobashi**, *National Institute of Advanced Industrial Science and Technology, Japan* | **Hidekazu Nishino**, *National Institute of Advanced Industrial Science and Technology, Japan* |**Takeo Yamada,** *National Institute of Advanced Industrial Science and Technology, Japan*| **Don Futaba**, *National Institute of Advanced Industrial Science and Technology, Japan*| **Kenji Hata**, *National Institute of Advanced Industrial Science and Technology, Japan*

Carbon nanotubes have the highest Young's modulus and strength among any known material, expected as outstanding reinforcing fillers. Reinforcement of matrix with CNTs would be fulfilled by harnessing the high aspect ratio, the alignment, the large CNT-matrix interfacial area, and the effective interfacial stress transfer. High filling of CNTs further enhances the mechanical strength of the composites. Randomly dispersed CNT/epoxy composites were conventionally fabricated from CNT dispersions, resulting in moderate improvements in the mechanical properties at the low filling as well as shortening nanotubes. We present an aligned SWNT sheet with nanoporosity, gSWNT prepreg sheeth, which is an excellent template for resin filling, affording a high SWNT fraction. The SWNT sheet was made by direct use of the SWNT forest (roll-press) without dispersing and impairing nanotubes. These SWNTs are very long, aligned, catalyst free, with high surface area, and synthesized by water-assisted CVD gSuper-growthh. By controlling an epoxy filling process, it was found that the nanotube content can be tuned at 20-35 wt%, giving the Young's modulus of 15 GPa (5.4-fold enhancement). XRD patterns revealed that the alignment of nanotubes was kept after the epoxy filling. The nanotube alignment-dependent mechanical properties were confirmed which is indicative of an importance of alignment. Cross-sectional observation of the composite film showed that the nanotubes were well-dispersed on a nanoscale even at the high fraction. The thickness of composite films are controllable in the range of 20-40 micrometer. Thinner films had the higher nanotube fraction and the enhanced mechanical properties.

## 10:00-10:30 Coffee Break

## 10:01-11:30 Poster Session 1

**See pages 57-72**

**SESSION CHAIR: THOMAS PICHLER**, *University of Vienna*

## 11:30-11:55 Invited Talk 1

### Ab initio Quantum Transport in Carbon Nanostructures

**Jean-Christophe Charlier**, *University Of Louvain, Belgum*

Their unusual electronic and structural physical properties promote carbon nanostructures as promising candidates for a wide range of nanoscience and nanotechnology applications. Not only can carbon 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 and graphene nanoribbons, as controlled by their topology, allows us to build logic devices at the nanometer scale, as already demonstrated in many laboratories. The goal of the present talk is to illustrate how ab initio modeling can help to predict the quantum transport properties in these carbon-based nanostructures. More specifically, the effect of realistic defects on the sensing ability of carbon nanotubes will be presented. The electronic and the magnetic properties of nanotubes decorated with metallic clusters will also be proposed. At last, the spin-polarized density functional theory will be used to investigate the electronic and transport properties of graphene nanoribbons with various edges geometries and topological disorder.

## 11:55-12:12 Contributed Talk 4

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

**Annick Loiseau**, *LEM, Onera-Cnrs, France* | **Hong Lin**, *LEM, Onera-Cnrs, France; MPQ, Université Paris Diderot - CNR, France* | **J erome Lagoute**, *MPQ, Université Paris Diderot - CNR, France* | **Raul Arenal**, *LEM, Onera-Cnrs, France* | **Vincent Repain**, *MPQ, Université Paris Diderot - CNR, France* | **Toma Susi**, *NMG, Department of Applied Physics, Aalto University, Finland* | **Esko Kauppinen**, *NMG, Department of Applied Physics, Aalto University, Finland* | **Sylvie Rousset**, *MPQ, Université Paris Diderot - CNR, France*

We have studied the impact of nitrogen atoms on the electronic structure of C-SWNTs by combining STM/STS and TEM/EELS. To this aim, CNx-SWNTs have been synthesized by two different techniques, the vaporization with a continuous laser of a C:Ni/Y target under a nitrogen atmosphere [1] and a CVD floating catalyst reactor using a hot iron wire/CO/ammonia system [2]. General common features emerge from the investigations of both kinds of samples. First, EELS analysis indicates a mean nitrogen concentration centered on 1 at.% but with significant variations from one tube to the other. Fine structure of absorption edges reveal the existence of two different local environments of N atoms. The first one is the graphitic configuration where an N atom is simply substituted to a C atom but is sporadically observed. The major configuration defines a more complex configuration involving pyridinic-like nitrogen atoms. STM/STS reveal the presence of specific defects which can been assigned to the presence of N atoms as they are not observed in pure C-SWNTs analogs. They give rise, in images, to different protusions extended over 3-5 nm exhibiting interference patterns and in spectroscopy, to the occurrence of different kinds of localized states, which will be discussed. These signatures indicate different kinds of N configuration in agreement with EELS. [1] H. Lin et al, J. Phys. Chem. C, 113, 9509 (2009) [2] T. Susi et al, Physica Status Solidi B (2009)

## 12:12-12:29 Contributed Talk 5

### Bump watch: sorting out metallic from semiconducting carbon nanotubes

**Ana Paula Barboza**, *Universidade Federal De Minas Gerais, Brazil* | **Ana Paula Gomes**, *Universidade Federal De Minas Gerais, Brazil* | **Helio Chacham**, *Universidade Federal De Minas Gerais, Brazil* | **Bernardo Neves**, *Universidade Federal De Minas Gerais, Brazil*

Single-wall carbon nanotubes (SWCTs) have been considered as possible materials to be used in future nano-electronic and nano-fluidic devices. In order to achieve such goals, a complete separation of metallic from semiconducting SWNTs is necessary, as they are normally produced in a random mixture of both types. Several routes for exclusive growth of one type or the other have been proposed, with some encouraging success. Nevertheless, even within such recipes, the labeling of metallic and semiconducting specimens on a typical production sample is a major bottleneck, as the conventional labeling techniques, such as Raman or I(V) characterization can only be applied to one SWNT at a time and, in most conditions, cannot be applied to any nanotube on the sample. In this work, we propose a new methodology to directly distinguish the electric nature of any SWNT on a typical as-grown process-free sample. It relies on the differences of the electric response of metallic and semiconducting SWNTs to a DC electric field applied by an Electric Force Microscopy (EFM) tip. Therefore, conventional EFM images directly single out the electric character of every and each nanotube by showing that not only the magnitudes of their response are different, but, more importantly, the EFM line profile across a nanotube is qualitatively distinct for metallic or semiconducting SWNTs. Theoretical modeling successfully explains and fit the experimental data, giving support to this very simple, yet extremely accurate and all-encompassing methodology.

**SESSION CHAIR: TOBIAS HERTEL**, *University of Würzburg*

## 14:00-14:25 Invited Talk 2

### New concepts in molecular and energy transport within carbon nanotubes: thermopower waves, stochastically resonant ion channels, and single molecule biosensors

**Michael Strano**, *Massachusetts Institute of Technology, USA*

Our laboratory has been interested in how carbon nanotubes can be utilized to illustrate new concepts in molecular and energy transfer. In the first example, we predict and demonstrate the concept of thermopower waves for energy generation. Coupling an exothermic chemical reaction with a thermally conductive CNT creates a self-propagating reactive wave driven along its length. We realize such waves in MWNT and show that they produce concomitant electrical pulses of high specific power >7 kW/kg. Such waves of high power density may find uses as unique energy sources. In the second system, we fabricate and study SWNT ion channels for the first time and show that the longest, highest aspect ratio, and smallest diameter synthetic nanopore examined to date, a 500 µm SWNT, demonstrates oscillations in electro-osmotic current at specific ranges of electric field, that are the signatures of coherence resonance, yielding self-generated rhythmic and frequency locked transport. The observed oscillations in the current occur due to a coupling between stochastic pore blocking and a diffusion limitation that develops at the pore mouth during proton transport. Lastly, I will discuss our work on biosensors based on SWNT fluorescence, which has advanced such that we can develop platforms to solve longstanding biological problems. Here, we develop an array of fluorescent SWNT that selectively record the discrete, stochastic quenching events that occur as H2O2 molecules are emitted from individual human epidermal carcinoma cells. We use this sensor array to map, for the first time, the H2O2 signaling pathway.

## 14:25-14:42 Contributed Talk 6

### Nanotube point defects and their physiochemical effects

**Philip G. Collins**, *Univ. Of California, USA* | **Vaikunth R. Khalap**, *Univ. Of California, USA* | **Steven R Hunt**, *Univ. Of California, USA* | **Israel Perez**, *Univ. Of California, USA* | **Tatyana Sheps**, *Univ. Of California, USA* | **Brad L. Corso**, *Univ. Of California, USA* | **Danny Wan**, *Univ. Of California, USA*

Single point defects can have disproportionate effects on the physiochemical properties of single walled nanotubes. We have developed a suite of experimental techniques for producing defects singly, identifying them, and characterizing their effects in single, isolated nanotubes. By investigating the same nanotube before and after defect incorporation, we conclusively determine the physiochemical consequences of different surface chemical modifications. For example, the added electrical resistance of a single ether modification is relatively subtle and at least one hundredfold less than for one carboxylate. Scanning probe microscopy spatially resolves this resistance, and probes its sensitivity to local gating. Alternately, electrochemical cycling of a nanotube in an electrolyte allow quantitative determination of the enhanced interfacial electron transfer rates associated with a particular defect type. This fundamental characterization is augmented by chemical manipulation of point defects as scaffolding sites for the attachment of fluorophores, catalytically active nanoclusters, and biomolecules. Each case provides new insights into the mechanisms underlying anticipated nanotube applications, and identifies surface chemistries responsible for different effects reported in the nanotube literature.

## 14:42-14:59 Contributed Talk 7

### Electron dynamics in carbon nanotubes with confining defects

**Gilles Buchs,** *Kavli Institute Of Nanoscience Delft, Netherland* | **Dario Bercioux**, *Physikalisches Institut and Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universitä, Germany* | **Oliver Groening**, *EMPA Swiss Federal Laboratories for Materials Testing and Research, Switzerland* | **Hermann Grabert**, *Physikalisches Institut and Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universitä, Germany*

Recently, carbon nanotubes have emerged as a very promising alternative to semiconducting systems for the realization of quantum dots (QD). In particular, single walled carbon nanotubes (SWCTs) with a controlled number of local defects give rise to QDs with level spacing much larger than the thermal energy at room temperature. Such devices are of considerable interest regarding applications in nanoelectronics, nanophotonics and quantum information/computation. We have investigated standing waves in intratube QDs created in metallic SWNTs using medium energy Ar+ ions irradiation. This technique permits the realization of ultra short (< 10 nm) intra-tube QDs showing particle-in-a-box states with level spacings of the order of 200 meV. To analyse defect-induced electron scattering, we have combined the Fourier-transform scanning tunnelling spectroscopy technique with the results of a Fabry-Perot electron resonator model. Within this approach we show the different contributions from inter- and intra-valley scattering of electrons confined between consecutive irradiation-induced defects. Our main result is the observation of coherent electron scattering among all six Dirac cones of the first Brillouin zone of the unrolled graphene structure [1]. This effect is attributed to the lack of translational invariance along the SWNT axis induced by the scattering defects. We further observe selection rules ascribable to the interplay between the tube and the defect symmetry [2]. [1] G. Buchs et al., Phys. Rev. Lett. 102, 245505 (2009) [2] D. Bercioux et al., in preparation

## 14:59-15:16 Contributed Talk 8

### Vapor Sensors Using Olfactory Proteins Coupled to Carbon Nanotubes

**Brett Goldsmith**, *University Of Pennsylvania, USA* | **Mitchell Lerner**, *University Of Pennsylvania, USA* | **Joe Mitala**, *University Of Pennsylvania, USA* | **Bohdana Discher**, *University Of Pennsylvania, USA* | **A.T. Charlie Johnson**, *University Of Pennsylvania, USA*

We have constructed bio-nano devices which combine mammalian olfactory proteins with carbon nanotubes to create a new class of vapor sensors. Olfactory proteins are a specific class of G-protein coupled receptors, and require a cell membrane or similar environment for proper function. Functionalization procedures have been developed to meet the challenges of routinely coupling such membrane proteins to nanotubes, while preserving the function of the protein. We have successfully isolated olfactory proteins and attached them to carbon nanotube transistors, which provide fast, all-electronic readout of analyte binding by the olfactory receptor. Several different olfactory proteins have been tested, each showing a different sensing response. This work opens the way for future coupling of biology to nanoelectronics and improved biomimetic chemical sensing. This work is supported by the DARPA RealNose Project and the Nano/Bio Interface Center

## 15:16-15:33 Contributed Talk 9

### First Experimental Observation of Single-File Water Transport into Single-Wall Carbon Nanotubes

**Sofie Cambré**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Bob Schoeters**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Sten Luyckx**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Wim Wenseleers**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium* | **Etienne Goovaerts**, *Physics Department, University of Antwerp (campus Drie Eiken), Belgium*

Single-file water filling of carbon nanotubes is observed for the first time,[1] through the splitting of the radial breathing mode (RBM) vibration in aqueous solution Raman spectra, when both empty (closed) and water-filled (open-ended) tubes are present. The narrow RBM linewidth needed to resolve this effect[2] is achieved by using bile salt surfactants (deoxycholate)[3], which yield a very homogeneous monolayer coating of the SWNTs. Filling with water is observed for a wide range of diameters, down to extremely thin tubes (e.g. (5,3) tube, diameter = 0.548nm) for which only a single water molecule fits in the cross-section of the internal nanotube channel.[1] The shift in RBM frequency upon filling is found to display a very complex, non-monotonic dependence on nanotube structure, in support of a different yet well-defined ordering of water molecules at room temperature, depending critically on nanotube diameter and chirality. Large shifts of the electronic transitions are also observed. [1] S. Cambré, B. Schoeters, S. Luyckx, E. Goovaerts & W. Wenseleers. 'Experimental Observation of Single-File Water Filling of Thin Single-Wall Carbon Nanotubes down to Chiral Index (5,3)' (to be published). [2] W. Wenseleers, S. Cambré, J. Culin, A. Bouwen & E. Goovaerts. 'Effect of water filling on the electronic and vibrational resonances of carbon nanotubes: Characterizing tube opening by Raman spectroscopy' Adv. Mater. 19, 2274-2278 (2007). [3] W. Wenseleers, I.I. Vlasov, E. Goovaerts, E.D. Obraztsova, A.S. Lobach & A. Bouwen. 'Efficient isolation and solubilization of pristine single-walled nanotubes in bile salt micelles' Adv. Funct. Mater. 14, 1105-1112 (2004).

## 15:30-16:00 Refreshment Break

## 15:33-17:00 Poster Session 2

**See pages 73-89**

**SESSION CHAIR: ADO JORIO**, *ICEx*

## 17:00 17:25 Invited Talk 3

### Exciton environmental effect of single wall carbon nanotubes

**Riichiro Saito**, *Tohoku University, Japan* | **Ahamad R. T.Nugraha**, *Tohoku University, Japan* | **Kentaro Sato**, *Tohoku University, Japan* | **Ado Jorio**, *Universidade Federal de Minas Gerais* | **Paul T. Araujo**, *Universidade Federal de Minas Gerais* | **Gene Dresselhaus**, *MIT* | **Mildred S. Dresselhaus**, *MIT*

Optical transition energies of single wall carbon nanotubes (SWNTs) are given by bright exciton energies. Because of relatively large exciton binding energy, exciton phenomena is essential for SWNTs even at room temperature. Because of low dimensionality, the exciton binding energy depends on the surrounding materials, which we call exciton environmental effect. In order to reproduce the transition energies observed in the experiment for a large region of diameter or energy and for a many varieties of surrounding materials, we propose a simple function of dielectric constant for an exciton binding calculation. From this, we can obtain the transition energies for any environments, which is useful for (n,m) assignment from the experiment.

## 17:25-17:42 Contributed Talk 10

### Resonance Raman Studies of Chirality-Enriched Single-Walled Carbon Nanotubes

**Stephen Doorn**, *Los Alamos National Laboratory, USA* | **Juan Duque**, *Los Alamos National Laboratory, USA* | **Erik Haroz**, *Dept. of Electrical and Computer Engineering, Rice University* | **Hang Chen**, *Dept. of Electrical and Computer Engineering, Boston University* | **Anna Swan**, *Dept. of Electrical and Computer Engineering, Boston University*

Probing chirality-defined electronic behaviors uniquely accessible through resonance Raman of the nanotube G-band requires working at either the single tube level or with ensemble samples highly enriched in a single type of tube structure. We present Raman measurements on such enriched ensemble samples from strategies employing both density gradient ultracentrifugation (DGU) and DNA wrapping-based ion chromatography. We provide Raman evidence for DGU enrichment of armchair metallic chiralities. Coupling of the G-band to low-energy excitations near the Fermi level in metallic nanotubes is important in defining transport behavior. G-band data for spectroscopically isolated armchair chiralities show that the relevant low-frequency LO mode is absent for these structures, in contrast with recent theoretical results. We also present resonance window behavior of G-band spectra for several single chirality semiconducting species. The Raman excitation profiles at resonance with the E22 transitions allow testing of different models for the Raman scattering process. Strong asymmetries in the profiles reveal new evidence for the importance of non-Condon effects in the Raman response. Results will be discussed in the context of theoretical models that suggest significant coordinate dependence in the transition dipole and phonon-mediated state mixing. Quantum interference between the higher lying E33 and E44 transitions for selected chiralities is also probed using UV resonance Raman at energies up to 3.6 eV. The novel behaviors of relative LO and TO mode intensities and their excitation profiles are discussed in terms of both Raman interference effects and state mixing.

## 17:42-17:59 Contributed Talk 11

### Phase transformations of bundles of SWNT, DWNT and peapods under extreme conditions. Contribution to carbon composite engineering

**Caillier Christophe**, *University of Lyon 1 and CNRS, France* | **Acrisio Aguiar**, *University of Lyon 1 and CNRS, France; University Federal of Ceara, Fortaleza, Brazil* | **Alexandre Merlen**, *University of Lyon 1 and CNRS, France; University Sud Toulon-Var, France* | **Antonio Gomes Souza Filho**, *University Federal of Ceara, Fortaleza, Brazil* | **Edouardo Bede Barros**, *University Federal of Ceara, Fortaleza, Brazil* | **Denis Machon**, *University of Lyon 1 and CNRS, France* | **Sylvie Le Floch**, *University of Lyon 1 and CNRS, France* | **Rodrigo Capaz**, *Universidade Federal do Rio de Janeiro, Brazil* | **Alfonso San Miguel**, *University of Lyon 1 and CNRS, France*

SWNT, DWNT and peapopds have been studied in situ under high pressure and high temperature conditions up to maximum values of 40 GPa and 1800 K using Raman spectroscopy and TEM and theoretically through ab initio calculations. The pressure induced transformations include the nanotube collapse, graphitization and transformation into diamond which were observed in situ or after sample recovering. At ambient temperature, the volume collapse of the SWNT takes place at pressures ranging from 10 GPa to higher than 40 GPa depending on the nature of the carbon nanotube matrix environment. We have observed that the filling of SWNT strongly modifies the collapse pressure. In particular homogeneous filling, as filling with argon or with another tube (DWNT) contributes to the stability of the tubes in good agreement with calculations. On the contrary, inhomogeneous filling, as in the case of peapods, decreases the system mechanical stability. Depending on the loss of hydrostatic conditions or on the combined application of pressure and temperature, partial or total graphitization is observed associated with the collapsed structure. For pressures of 14.5 GPa and temperatures of 1800 K the nanotubes are irreversibly transformed into cubic diamond. On the basis of our results, we discuss possibilities for new carbon–carbon composite engineering from carbon nanotube bundles.

## 17:59-18:16 Contributed Talk 12

### Tribute to Peter C. Eklund

**Mildred Dresselhaus**, *Massachusetts Institute Of Technology, USA*

# Wednesday, June 30

**SESSION CHAIR: PHILIP KIM**, *Columbia University*

## 8:30-9:10 Keynote 2

### Carbon in Two Dimensions: Magic of Graphene

**Andre Geim**, *University of Manchester, United Kingdom*

Graphene has turned out to be a wonder material adding new dimensions to research on nanotubes and their applications. Similar to the latter, graphene has already attracted many superlatives to its name. It is of course the thinnest material imaginable and arguably the strongest one ever measured. Its charge carriers exhibit the highest intrinsic mobility, have zero effective mass and can travel micron distances without scattering at room temperature. Graphene can sustain current densities million times higher than copper, shows record thermal conductivity and stiffness, is impermeable to gases and reconciles such conflicting qualities as brittleness and ductility. Electron transport in graphene and its bilayer is described by massless and massive Dirac-like equations, respectively (rather than the standard Schrodinger equation), which allows the investigation of relativistic quantum phenomena in a bench-top experiment. Some of graphene's superlatives and phenomena have paralleled those known for carbon nanotubes but others are strictly due to the two dimensional nature of graphene. I will overview our work on graphene concentrating on its fascinating electronic and optical properties, and using for illustration mostly the results obtained by our group in Manchester. In addition, I will attempt to describe the rapidly developing area of graphene applications. For review, see A. K. Geim, Science 324, 1530 (2009). A. K. Geim, K. S. Novoselov, Nature Mater. 6, 183 (2007).

## 9:10-9:27 Contributed Talk 13

### Low-temperature synthesis of graphene by chemical vapor deposition and fabrication of top-gated transistors using transfer-free processes

**Daiyu Kondo**, *Nanoelectronics Research Center, Fujitsu Laboratories Ltd., Japan* | **Shintaro Sato**, *Nanoelectronics Research Center, Fujitsu Laboratories Ltd., Japan* | **Katsunori Yagi**, *Nanoelectronics Research Center, Fujitsu Laboratories Ltd., Japan* | **Naoki Harada**, *Nanoelectronics Research Center, Fujitsu Laboratories Ltd., Japan* | **Naoki Yokoyama**, *Nanoelectronics Research Center, Fujitsu Laboratories Ltd., Japan*

Graphene has been attracting attention as one of promising materials utilized in the future electronic devices due to its superb physical and structural properties since the first report on its isolation[1]. Many studies regarding graphene devices have been performed using graphene exfoliated from graphite. Recently, studies on graphene synthesis by chemical vapor deposition (CVD) and its transfer to other substrates for device fabrication have been reported[2, 3]. However, such a transfer process may not be appropriate for applications using a large substrate, including large-scale integrated circuits. In this study, we demonstrate synthesis of graphene at a temperature of 650°C, which is lower than those reported previously and propose a novel method to fabricate graphene-channel top-gated field-effect transistors (FETs) directly on a SiO2/Si substrate without using transferring processes[4]. Few-layer and multi-layer graphene was synthesized by thermal CVD with acetylene as the source gas. Iron films were used as catalyst. We found that the thickness of graphene depends on the catalyst thickness and the supply of the source gas. For device fabrication, graphene was synthesized on patterned iron films. The iron was subsequently etched after both ends of the graphene were fixed by two electrodes, leaving the graphene channels bridging the electrodes all over the substrate. Top-gated FETs were then made after covering the channels with HfO2. The fabricated devices exhibit ambipolar behaviour and can sustain a high-density current. [1] Science 306 (2004) 666. [2] Nano Lett. 9 (2009) 30. [3] Nature 457 (2009) 706. [4] Appl. Phys. Express 3 (2010) 025102.

## 9:27-9:44 Contributed Talk 14

### Energy Transfer from Individual Semiconductor Nanocrystals to Graphene

**Zheyuan Chen**, *Columbia University* | **Stéphane Berciaud**, *Columbia University* | **Colin Nuckolls**, *Columbia University* | **Tony Heinz**, *Columbia University* | **Louis Brus**, *Columbia University*

Energy transfer from photoexcited zero-dimensional systems to metallic systems plays a prominent role in modern day materials science. A situation of particular interest concerns the interaction between a photoexcited dipole and an atomically thin metal. The recent discovery of graphene layers permits investigation of this phenomenon. Here we report a study of fluorescence from individual CdSe/ZnS nanocrystals in contact with single- and few-layer graphene sheets. The rate of energy transfer is determined from the strong quenching of the nanocrystal fluorescence. For single-layer graphene, we find a rate of ~ 4ns-1, in agreement with a model based on the dipole approximation and a tight-binding description of graphene [1]. This rate increases significantly with the number of graphene layers, before approaching the bulk limit. Our study quantifies energy transfer to and fluorescence quenching by graphene, critical properties for novel applications in photovoltaic devices and as a molecular ruler. References: [1] R.S. Swathi and K.L. Sebastian, J. Chem Phys. 129, 054703 (2008) [1] R.S. Swathi and K.L. Sebastian, J. Chem Phys. 130, 086101 (2009) [2] Z. Chen et al. arXiv:1003.3027v1

## 9:44-10:01 Contributed Talk 15

### Can Graphene be used as a Substrate for Raman Enhancement?

**Xi Ling**, *Center of Nanochemistry, College of Chemistry and Molecular Engineering, China* | **Jin Zhang**, *Center of Nanochemistry, College of Chemistry and Molecular Engineering, Peking University, China* | **Zhongfan Liu**, *Center of Nanochemistry, College of Chemistry and Molecular Engineering, Peking University, China* | **Mildred S. Dresselhaus**, *Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, USA* | **Jing Kong**, *Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, USA*

Here, we discussed the possibility that graphene can be used as a substrate for enhancing Raman signals of adsorbed molecules. First, the fluorescence background of the molecule was observed suppressed by graphene substrate. Furthermore, by comparing the Raman signals of molecule on graphene and on a SiO2/Si substrate, Raman enhancement effect was found existent on the surface of graphene. The Raman enhancement factor of 2-17 was found dependent on the symmetry of vibrations of the molecule. The enhancement efficiency was much remarkable for few-layer graphene. Based on the Raman enhancement effect on graphene, the adsorption ability was proved change oscillated with every second layers, which is related with the electron concentration on the surface of graphene. Besides, the Raman enhancement effect was confirmed also by depositing the molecule before graphene transferring (the molecule on the bottom of graphene). The intensity of the Raman signals from the molecule was obviously different for the molecule on top (or bottom) of graphene, which was proved dependent on the molecular configuration by depositing the molecule with a certain orientation using the Langmuir-Blodgett technique. Both the theoretical analysis and the experimental data show the Raman enhancement on graphene belongs to the chemical enhancement mechanism. References: 1. L. M. Xie, X. Ling, Y. Fang, J. Zhang, and Z. F. Liu, JACS, 131, 2009, 9890-9891 2. X. Ling, L. Xie, Y. Fang, H. Xu, H. Zhang, J. Kong J, M. S. Dresselhaus, J. Zhang , Z. F. Liu, Nano Letters, 10(2), 2010, 553-561

## 10:00-10:30 Coffee Break

## 10:01-11:30 Poster Session 3

**See pages 90-110**

**SESSION CHAIR: RALPH KRUPKE**, *Karlsruhe Institute of Technology*

## 11:30-11:55 Invited Talk 4

### Synthesis and characterization of doped SWNTs and graphitic nanoribbons

**Jessica Campos Delgado**, *Instituto Nacional De Metrologia, Normalização E Qualidade Industrial, Brazil* | **Mildred Dresselhaus**, *Massachusetts Institute of Technology* | **Humberto Terrones**, *Sociedad Mexicana de Nanociencias y Nanotecnología* | **Mauricio Terrones**, *Universidad de las Americas*

Carbon nanostructures come in many flavors: fullerenes, nanotubes, onions, nanohorns, toroids, graphene, nanoribbons, etc. In particular, carbon nanotubes have attracted a lot of attention due to their amazing electronic properties. We have been able to synthesize N-, P- and Si- doped SWNTs using an aerosol-assisted chemical vapor deposition technique. This method allows us to produce pristine SWNTs using ferrocene (Fe(C5H5)2) – ethanol (C2H6O) solutions. Doping elements are introduced to the CVD system by means of precursor compounds at different concentrations. Benzylamine (C7H7NH2), pyrazine (C4H4N2), triphenylphosphine ((C6H5)3P), methoxytrimethylsilane (CH3OSi(CH3)3), and thiophene (C4H4S) were the precursors used in this work. We have successfully produced N-, P- and Si- doped SWNTs. Our experiments with low concentrations of thiophene triggered the synthesis of a new carbon nanostructure: graphitic nanoribbons. The nanoribbons were annealed up to 2800 °C in graphitic furnaces. Our TEM observations revealed that under heat treatments a crystallization process occurs, and above 1500 °C, the adjacent graphitic sheets of the nanoribbons find a more stable configuration by forming loops. Single, double and multiple loops are formed at different stages of the heat treatments. Joule heating experiments of the nanoribbons were also carried out. Our results show that an intense irradiaton of the electron beam, prior to the experiment, results in the formation of sharp zigzag and armchair edges; while the experiment of an as-produced nanoribbon results in multiple-loop formation due to the high temperatures that are achieved in the experiment.

## 11:55-12:12 Contributed Talk 16

### Holographic valence charge mapping and evidence of a potential trap depression in graphene membranes and carbon nanotubes

**Luca Ortolani**, *CNR IMM-Bologna, Italy* | **Florent Houdellier**, *CNRS CEMES, France* | **Etienne Snoeck**, *CNRS CEMES, France* | **Marc Monthioux**, *CNRS CEMES, France* | **Vittorio Morandi**, *CNR IMM-Bologna, Italy*

The band structure of graphene presents six conical points where the energy dispersion is perfectly linear in the momentum. This particular feature is at the basis of the interesting physical and chemical properties of this material. Upon stacking to form a Few-Graphene-Crystal (FGC), the interlayer interaction induce a small valence charge redistribution in the crystal lattice, suppressing the linear dispersion in the band-structure. In particular, in turbostratic FGCs for certain orientations, when the lattices are commensurable, graphenes electronically decouple, and the FGC behaves like an individual monolayer. Using transmission electron holography, we investigated the redistribution of electronic crystal charges in a commensurate turbostratic FGC, in which the number of layers varies from an individual graphene up to four. Using the same technique we probed the charge distribution in individual CNTs as the number of walls decreases from 20 down to a single-walled (SW-)CNT. The phase investigation of the turbostratic, non commensurate stacking of graphenes in concentric multi-walled (MW-)CNTs revealed a size effect originating from the charge redistribution in the under-coordinated surface graphene. The data shows an increase of the phase shift, hence a depression of the average atomic potential traps, as the proportion of surface atoms over the total number of atoms for an individual nanotube decreases. Comparing electron phase shifts of a FGC and CNTs, we found that the commensurate stacking geometry makes each graphene in the FGC be decoupled from any neighboring graphene, shifting the electron phase as a surface (individual) graphene does.

## 12:12-12:29 Contributed Talk 17

### Tunable bandgaps and excitons in doped semiconducting carbon nanotubes made possible by acoustic plasmons

**Catalin Spataru**, *Sandia National Laboratories, USA* | **François Léonard**, *Sandia National Laboratories, USA*

Doping of semiconductors is essential in modern electronic and photonic devices. While doping is well understood in bulk semiconductors, the advent of carbon nanotubes and nanowires for nanoelectronic and nanophotonic applications raises some key questions about the role and impact of doping at low dimensionality. Here we show that for semiconducting carbon nanotubes, bandgaps and exciton binding energies can be dramatically reduced upon experimentally relevant doping, and can be tuned gradually over a broad range of energies in contrast to higher dimensional systems. The later feature, made possible by a novel mechanism involving acoustic plasmons, establishes new paradigms for the understanding and design of nanoelectronic and nanophotonic devices.

**SESSION CHAIR: PHIL COLLINS**, *University of California Irvine*

## 14:00-14:42 Keynote 3

### Carbon nanotubes: from 'string' theory to solar energy

**Paul McEuen**, *Cornell U., USA*

Carbon nanotubes are remarkable materials, with properties midway between molecules and extended solids. Mechanically, nanotubes are stiff polymers, and we present measurements of their flexural and torsional bending properties. Electronically, nanotubes are quasi-one dimensional conductors with subbands that have both spin and orbital degrees of freedom. Here we report the observation of topological coupling between them due to the nanotube's cylindrical geometry. Finally, nanotube have remarkable optical properties. Here we present optoelectronic measurements of nanotube p-n junction photodiodes. We find ultra-efficient electron-hole pair production by high energy carriers, a process of great interest for next-generation solar cells.

## 14:42-14:59 Contributed Talk 18

### Detection of phase transitions in adsorbed layers on single-walled carbon nanotube nanobalances

**David Cobden**, *Department of Physics, University Of Washington, USA* | **Zenghui Wang**, *Department of Physics, University Of Washington, USA* | **Erik Fredrickson**, *Department of Physics, University Of Washington, USA* | **Oscar Vilches**, *Department of Physics, University Of Washington, USA*

Suspended single-walled carbon nanotubes can act as nanoscale resonators with remarkable electromechanical properties and the ability to detect adsorption at the level of single atoms. Understanding adsorption on nanotubes and other graphitic materials is key to many sensing and storage applications. We show that nanotube resonators offer a powerful new means of investigating fundamental aspects of adsorption on carbon, including the collective behavior of adsorbed matter and its coupling to the substrate electrons. By electrically monitoring the resonance frequency in the presence of noble gases at controlled pressure and temperature, we observe the formation of monolayers on the cylindrical surface and phase transitions within these monolayers. With krypton we see direct evidence for a commensurate solid coating the nanotube, raising interesting questions related to the cylindrical geometry and nanotube chirality. We also observe a change in the electrical conductance at a phase transition suggesting a modification of the bandgap by the adsorbate and allowing measurements of the dynamics of the transition. Finally, we study the modification of the phase transitions by current and gate voltage.

## 14:59-15:16 Contributed Talk 19

### Combined Raman and Electrical Transport Measurements on Individual, Ultra-Clean, Suspended SWNTs

**Steve Cronin**, *University of Southern California, USA* | **Adam Bushmaker**, *University of Southern California, USA* | **Vikram Deshpande**, *Columbia University, USA* | **I-Kai Hsu**, *University of Southern California, USA* | **Moh Amer**, *University of Southern California, USA* | **Chia-Chi Chang**, *University of Southern California, USA* | **Marc Bockrath**, *University of California, USA*

We report simultaneous Raman spectroscopy and electron transport measurements on individual carbon nanotubes. Our ability to fabricate nearly defect-free, ultra-clean, suspended single walled carbon nanotubes (SWCNTs) has enabled us to observe several interesting phenomena not seen before in carbon nanotubes, including breakdown of the Born-Oppenheimer approximation[1], mode selective electron-phonon coupling[2], and a Mott insulating behavior[3]. Raman spectroscopy of these nanotubes under applied gate and bias potentials reveals exceptionally strong electron-phonon coupling, arising from Kohn anomalies, which result in mode selective electron-phonon coupling, negative differential conductance (NDC), and non-equilibrium phonon populations[2,4]. Due to their long electron lifetimes, we observe a breakdown of the Born-Oppenheimer approximation, as deduced from the gate voltage-induced changes in the vibrational energies of suspended carbon nanotubes[1]. We also report large variations in the Raman intensity of metallic SWCNTs in response to gate voltages, which are attributed to a Mott insulating state of the strongly correlated electrons[3]. Lastly, the role of gas adsorption on thermal transport and hot phonon decay rates will also be discussed, as well as the effect of uniaxial strains as high as 13.7%. 1. Bushmaker, et al. Nano Letters, 9, 607-611 (2009). 2. Bushmaker, et al. Nano Letters, 7, 3618 (2007). 3. Bushmaker, et al. Physical Review Letters, 103, 067401 (2009). 4. Bushmaker, et al. Nano Letters, 9, 2862 (2009).

## 15:16-15:33 Contributed Talk 20

### An Extremely Black Thermal Detector

**John Lehman**, *NIST, USA* | **Aric Sanders**, *NIST, USA* | **Leonard Hanssen**, *NIST, USA* | **Boris Wilthan**, *NIST, USA* | **Christopher Jensen**, *SUNY, Stony Brook, USA*

In 2008 Yang et al. reported an extremely dark material made of carbon nanotubes. The authors cited our previous work and the application of carbon nanotubes for improved thermal-detector coatings. [Nano Letts, 8, 446-451, (2008); Appl. Opt. 45, 1093-1097, (2006)]. In this presentation we describe vertically aligned multiwall carbon nanotubes grown by water-assisted chemical vapor deposition on a large-area lithium tantalate pyroelectric detector. After coating, a cycle of heating, electric field poling and cooling was employed to restore the spontaneous polarization perpendicular to the detector electrodes. The detector responsivity is reported along with imaging as well as visible and infrared reflectance measurements of the detector and a silicon witness sample. We find nearly ideal values of detector reflectance uniformly less than 0.1 % from 400 nm to 4 µm and less than 1 % from 4 to 14 µm. At NIST and elsewhere, the basis of standards for measuring optical radiance, irradiance and the definition of the candela are based on a thermal detector of one sort or another. In nearly every case, these detectors have a black coating to enhance detection efficiency and spectral uniformity. Thus, our ability to make better coatings supports our ability to make more accurate measurements for a variety of NIST priorities such as optical fiber-based communication systems, photovoltaic and solar-thermal efficiency, satellite-based sensors for earth and sun temperature measurements and laser-based manufacturing. Our research demonstrates an immediate and practical application of carbon nanotubes.

## 18:00-23:00 Excursion and Banquet

# Thursday, July 1

**SESSION CHAIR: ESKO KAUPPINEN**, *Aalto University*

## 8:30-9:10 Keynote 4

### How does a single-walled carbon nanotube grow from a nanoparticle? The role of the catalyst in nanotube growth

**Yoshikazu Homma** , *Tokyo University Of Science, Japan*

Carbon nanotube and graphene are two of the materials attracting much attention currently. A single-walled carbon nanotube (SWNT) has a shape of rolled-up graphene, but growth process is quite different from that of graphene. While a large graphene sheet grows horizontally on a flat surface, a SWNT grows vertically on a curved surface of a nanoparticle. Transition metals can form either graphene or nanotube depending on the curvature. Interestingly, SWNTs are rather easy to grow if nanoparticles present, as if the chemical nature of the nanoparticle is unimportant: silicon, silicon carbide, alumina, and diamond as well as various metals including gold, silver, and copper act as the catalyst of SWNT growth. The physical shape, i.e., the curved surface with a high curvature might be necessary to form a cap structure with carbon pentagons, which would act as a nucleus of SWNT. Furthermore, the phase of the nanoparticle, either liquid or solid, may not be crucial. Still, the gcatalysth seems to have another role: supplying carbon atoms to the nanotube. Without catalyst particles, SWNTs rarely extend. This is also true for the growth of graphene edges. On the particle surface, carbon baring molecules might be converted to carbon atoms or other forms which can be incorporated into the edge of carbon hexagon networks. Recent progresses in SWNT growth would lead to better understanding of nanotube growth mechanism soon. Of great concern is the possibility of epitaxial growth of SWNTs from crystalline catalyst particles for chiral control of SWNTs.

## 9:10-9:27 Contributed Talk 21

### Catalytic Growth of Carbon Nanotube: Is the Size of Catalyst Determines the Diameter of Carbon Nanotube?

**Bilu Liu**, *Shenyang National Laboratory For Materials Science, Institute Of Metal Research,Chinese Academy of Sciences, China* | **Wencai Ren**, *Shenyang National Laboratory For Materials Science, Institute Of Metal Research,Chinese Academy of Sciences, China* | **Chang Liu**, *Shenyang National Laboratory For Materials Science, Institute Of Metal Research,Chinese Academy of Sciences, China* | **Bing Yu**, *Shenyang National Laboratory For Materials Science, Institute Of Metal Research,Chinese Academy of Sciences, China* | **Hui-Ming Cheng**, *Shenyang National Laboratory For Materials Science, Institute Of Metal Research,Chinese Academy of Sciences, China*

Single-walled carbon nanotubes (SWNTs) have attracted great deal of interests since their discovery. A SWNT can either be a semiconductor or metal, depend on its diameter and chiral angle. Furthermore, for those semiconducting ones, the band gaps are inversely proportional to their diameters. Therefore, the controlled synthesis of SWNTs with uniform diameters and chiral angles are critical for many practical applications. Abundant studies have suggested that the diameters of SWNTs were determined by the sizes of catalyst nanoparticles (NPs). However, the growth of small SWNTs from large catalyst NPs was also frequently observed. The diameter-controlled synthesis of SWNTs can only be fulfilled ground on unveiling the factors which can affect the diameters of SWNTs and know how they work. In this contribution, we employed high-resolution TEM transmission electron microscopy (HRTEM) and resonant Raman spectroscopy to study the catalyst size-SWNT diameter relationship in two chemical vapor deposition (CVD) processes, namely, supported catalyst and floating catalyst CVD processes. It is found that in a supported catalyst process, the as-grown SWNTs possess comparable diameters with the sizes of the Fe catalyst NPs; while the SWNT diameters constantly smaller than the catalyst sizes in floating catalyst process. An universal catalyst size-SWNT diameter relationship, which is suggested to be dependent on whether the catalyst is homogeneous or heterogeneous (both in chemical composition and in structural), is proposed based on our experiment results and that of others. These findings have potential to guide the diameter controlled synthesis of SWNTs.

## 9:27-9:44 Contributed Talk 22

### Gas-phase and On-surface Decomposition of Ethanol in Alcohol CVD

**Shigeo Maruyama**, *Dept. of Mechanical Engineering, The University Of Tokyo, Japan* | **Rong Xiang**, *Dept. of Mechanical Engineering, The University Of Tokyo, Japan* | **Bo Hou**, *Dept. of Mechanical Engineering, The University Of Tokyo, Japan* | **Erik Einarsson**, *Dept. of Mechanical Engineering, The University Of Tokyo, Japan* | **Junichiro Shiomi**, *Dept. of Mechanical Engineering, The University Of Tokyo, Japan*

We have previously investigated gas-phase thermal decomposition of ethanol and its effects on single-walled carbon nanotube (SWNT) synthesis by the alcohol catalytic CVD (ACCVD) method, and found that a significant fraction of ethanol quickly decomposes into various reactive byproducts such as C2H4, C2H2, and CH2. Calculations using the CHEMKIN software package were in good agreement with FT-IR measurements of chemical species detected in the gas ambient. However, the relative contribution of these species to SWNT growth remains unclear. To resolve this issue, we extended our analysis using isotopically modified ethanol, in which one of the carbons was 12C and the other 13C. Since ethanol is asymmetric the carbons are expected to contribute unequally to SWNT formation. After thermally decomposing into symmetric byproducts such as C2H4 and C2H2, the 12C and 13C contribution should be equal. The degree of contribution was determined from the isotope-induced shift in the Raman G-band frequency. We find the inequivalent contribution from ethanol varies with CVD parameters, and is more exaggerated at minimal decomposition conditions, e.g. low temperature and/or high flow rate. One unexpected finding, however, is that our data indicate that ethanol decomposition is also promoted by the presence of Mo on the substrate. This indicates that the role of Mo in ACCVD is not only to immobilize the Co catalyst, but also to promote local ethanol decomposition at the substrate surface. A model quantifying the gas-phase and surface decomposition processes will be proposed, and the effects on SWNT quality will be discussed.

## 9:44-10:01 Contributed Talk 23

### Single-walled carbon nanotube nucleation, growth and termination studied by in situ Raman measurements

**Vincent Jourdain**, *Université De Montpellier, France* | **Matthieu Picher**, *Université De Montpellier, France* | **Eric Anglaret**, *Université De Montpellier, France* | **Raul Arenal**, *LEM ONERA-CNRS, Châtillon, France*

Despite considerable progress in the control of the carbon nanotube length, orientation and structure, the fundamental processes involved in nanotube nucleation, growth and termination remain poorly understood. The complexity of the problem especially arises when one considers the different chemical and physical processes operating on surface and in gas phase, at different time and spatial scales. Develop realistic growth models clearly requires the combination of theoretical and simulation works with reliable in situ data. As other groups [1-2], we chose to investigate the SWCNT growth using in situ Raman measurements because SWCNTs provide intense and specific Raman spectra. We initiated a systematic study as a function of the growth conditions [3] and catalyst-precursor couples. From our observations, two conditions are required for the nanotube nucleation: the catalyst particle must be reduced and reach a critical carbon concentration. Once reduced, the catalyst particles rearrange quickly. The growth kinetics is generally limited by the carbon supply at the catalyst surface. The nanotube crystalline quality appears controlled by the kinetic equilibrium between the supply of carbon atoms and their surface diffusion/rearrangement. We observed two types of termination: a process dominant at high temperature and low carbon supply compatible with an Ostwald ripening of the particles and a process dominant at low temperature and high carbon supply compatible with a catalyst encapsulation by a carbon layer. 1. Kaminska et al., Nanotechnology (2007) 18, 165707 2. Chiashi et al., Chemical Physics Letters (2004) 386, 89 3. Picher et al., NanoLetters (2009) 9, 542

### 10:00-10:30 Coffee Break

### 10:01-11:30 Poster Session 4

**See pages 111-128**

**SESSION CHAIR: CHRISTOPHE VOISIN,** *École Normale Supérieure*

### 11:30-11:55 Invited Talk 5

**Quantum optics with carbon nanotubes**
**Atac Imamoglu**, *ETH Zurich, Switzerland* | **Ajit Srivastava**, *ETH Zurich, Switzerland* | **Christophe Galland**, *ETH Zurich, Switzerland* | **Andres Vargas**

Semiconducting carbon nanotubes (CNT) constitute a new paradigm for solid-state quantum optics. Recent photoluminescence, resonant light scattering and photon correlation measurements shed new light onto single nanotube exciton dynamics.

### 11:55-12:12 Contributed Talk 24

**Femtosecond four-wave-mixing spectroscopy of freely suspended and fully characterized single-wall carbon nanotubes**
**Pasi Myllyperkiö**, *Nanoscience Center, University of Jyväskylä, Finland* | **Olli Herranen**, *Nanoscience Center, University of Jyväskylä, Finland* | **Jyri Rintala**, *Nanoscience Center, University of Jyväskylä, Finland* | **Hua Jiang**, *Center for New Materials, Aalto University, Finland* | **Andreas Johansson**, *Nanoscience Center, University of Jyväskylä, Finland* | **Prasantha R. Mudimela**, *Center for New Materials, Aalto University, Finland* | **Zhen Zhu**, *Center for New Materials, Aalto University, Finland* | **Albert G. Nasibulin**, *Center for New Materials, Aalto University, Finland* | **Esko I. Kauppinen**, *Center for New Materials, Aalto University, Finland* | **Markus E. Ahlskog**, *Nanoscience Center, University of Jyväskylä, Finland* | **Mika Pettersson**, *Nanoscience Center, University of Jyväskylä, Finland*

We have characterized the individual properties of freely suspended single-wall carbon nanotubes, using both Raman spectroscopy and electron diffraction measurements in a transmission electron microscope. The two techniques give mutually independent routes to determine the chirality of the nanotube [1,2], which allows us to find the corresponding detailed band structure. With help of that knowledge we set up time-resolved (femtosecond) four-wave-mixing (FWM) measurements and show that it is possible to obtain fs-FWM signals from individual suspended semiconducting single-wall carbon nanotubes. These measurements are the first in the femtosecond regime and they open interesting perspectives for measurements of ultrafast dynamics and nonlinear optical response from individual nanotubes. Within this study we next intend to measure directly the vibrational coherence in nanotubes of known chirality. [1] J. Rintala et al., J. Phys. Chem. C 113 (2009) 15398. [2] H. Jiang et al., Carbon 45 (2007) 662.

### 12:12-12:29 Contributed Talk 25

**Optical gain in carbon nanotubes**
**Etienne Gaufrès**, *Institut d'Electronique Fondamental, France* | **Nicolas Izard**, *Institut d'Electronique Fondamental, France* | **Xavier Le Roux**, *Institut d'Electronique Fondamental, France* | **Delphine Marris-Morini**, *Institut d'Electronique Fondamental, France* | **Saïd Kazaoui**, *National Institute of Advanced Industrial Science and Technology (AIST),Japan* | **Eric Cassan**, *Institut d'Electronique Fondamental, France* | **Laurent Vivien**, *Institut d'Electronique Fondamental, France*

Carbon nanotubes are a promising material for nanophotonics and optoelectronics. Since the discovery of nanotubes' photoluminescence upon encapsulation into micelle surfactant, research efforts in the nanotube photonic field have greatly intensified. Thanks to their excitonic recombination across a direct band gap, semiconducting nanotubes (s-SWNT) can be used as efficient light emitters in the near-IR. However, several non-radiative mechanisms existing in raw carbon nanotubes seriously quench their emission efficiency, which was up to now a major hindrance to potential applications. We report the first experimental demonstration of a room temperature 190 cm-1 intrinsic gain at 1300nm in a thin layer film containing only s-SWNT. We will first show in this talk that s-SWNTs without remaining traces of metallic nanotubes (m-SWNT) or catalyst particles could be extracted using an ultra-centrifugation process assisted by a polyfluorence (PFO) polymer. The evolution of s-SWNT optical properties as a function of m-SWNT concentration, studied by photoluminescence, absorption and Raman spectroscopy, will be presented. We will show that the purification enhance the emission and limit the optical losses in the thin layer film.We will present strong evidences for optical gain in (8,6) et (8,7) s-SWNT. We will also show that optical gain could not be achieved in a raw or lowly semiconducting-enriched sample due to interactions with the remaining m-SWNT. This result constitute a significant milestone towards the development of carbon nanotube based laser sources, and open promising perspectives for future high performance integrated circuits.

**SESSION CHAIR: SHIGEO MARUYAMA**, *University of Tokyo*

### 14:00-14:25 Invited Talk 6

**Preferential growth of single-walled carbon nanotubes with metallic conductivity**
**Avetik Harutyunyan**, *Honda Research Institute, USA*

The lack of reasonably homogeneous single walled carbon nanotube (SWCNT) materials hinders their ubiquitous applications. There have been significant achievements in separating and, thereby, enriching SWCNT materials according to their conductivity. Meanwhile, despite numerous studies there is only limited hints regarding the direct control over carbon nanotube structure during growth, and poor understanding of features that determine its chirality and, thereby, the electronic structure. Our in situ environmental transmission electron microscopy observations of the $SiO_2$ supported Fe nanocatalysts, which are suitable for nanotube nucleation, in various gaseous environments $H_2O$, $H_2/H_2O$, $Ar/H_2O$ and $He/H_2O$ reveal that presence of Ar in the ambient leads to significant coarsening of nanocatalysts with rounded surface morphology, while under He ambient the nanocatalyst is more faceted. Furthermore, we found that the variation of the noble gas ambient during thermal conditioning of the catalyst, in combination with oxidative and reductive species, alters the fraction of grown tubes with metallic conductivity from about 20% of the population to a maximum of 91%. Various scenarios such as adsorption and roughening induced morphology rearrangements of the catalyst particles and their relationships with grown tubes electronic structures will be presented.

### 14:25-14:42 Contributed Talk 26

**Catalyst recycling behavior in spinnable CNT synthesis**
**Chi Huynh**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia; Department of Materials Engineering, Monash University, Clayton, Victoria, Australia* | **Stephen Hawkins**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **Bill Humphries**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **Marta Redrado**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **Matthew Glenn**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **Scott Barnes**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **Thomas Gengenbach**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **Deborah Lau**, *Commonwealth Scientific and Industrial Research Organization (CSIRO), Australia* | **George Simon**, *Department of Materials Engineering, Monash University, Clayton, Victoria, Australia*

Carbon nanotubes have exceptional physical properties. Some can be spun directly from the growth substrate into a continuous pure web or yarn, which is of great technological and theoretical interest. Although an extremely sensitive process, particularly with respect to catalyst structure and behaviour, we have achieved reliable synthesis of spinnable CNTs using acetylene. A recycling methodology has been developed that allows the catalyst (iron) to be analysed incrementally. It also gives us the capacity to control the resultant CNT and hence yarn and web properties.  The catalyst remains bound to the substrate and able to regrow CNTs >7 times. The first four cycles are spinnable when grown with acetylene alone, or, with hydrogen, the first two cycles. Striking changes to the catalyst and CNT properties occur with recycling and the addition of hydrogen.  Acetylene alone gives a steady yield for four cycles before declining sharply on the fifth; diameter steadily decreases, whilst areal density rises after the fourth cycle. Hydrogen initially gives larger catalyst particles and higher areal density (2.20x1011 tube/cm2) compared with acetylene alone (1.32x1011 tube/cm2), twice the growth rate and smaller diameter (8.7 vs. 10.5 nm). Yield drops dramatically for the third and subsequent cycles, mean diameter then gradually increases and areal density declines. Overall yield for the two approaches is nevertheless about equal.  Detailed analysis (by AFM, XPS, HRTEM) of the substrate shows extensive catalyst restructuring (with contrary effects when hydrogen is added) which occurs due to the reaction process, rather than the cumulative effect of heating.

## 14:42-14:59 Contributed Talk 27

### Green nanotubes: very high quality single-walled carbon nanotubes synthesized from biologically renewable carbon

**Christopher Kingston**, *National Research Council Canada, Steacie Institute for Molecular Sciences, Canada* | **Michael Jakubinek**, *National Research Council Canada, Steacie Institute for Molecular Sciences, Canada* | **Yadienka Martinez-Rubi**, *National Research Council Canada, Steacie Institute for Molecular Sciences, Canada* | **Jingwen Guan**, *National Research Council Canada, Steacie Institute for Molecular Sciences, Canada* | **Patricia Grinberg**, *National Research Council Canada, Institute for National Measurement Standards* | **Ralph Sturgeon**, *National Research Council Canada, Institute for National Measurement Standards* | **Benoit Simard**, *National Research Council Canada, Steacie Institute for Molecular Sciences, Canada*

All current methods for the production of single-walled carbon nanotubes (SWCNT) use carbon feedstock derived from petrochemical or other synthetic sources. As applications for SWCNT continue to mature and usage continues to expand, the production of SWCNT will add additional strain on global petrochemical resources. The use of renewable carbon feedstock will allow the full potential of SWCNT to be realized without impacting existing energy resources. We have successfully synthesized very high purity SWCNT from BioChar [Dynamotive], a biologically renewable carbon source produced as a co-product of the fast pyrolysis of cellulosic biomass for BioOil production. The BioChar was processed into target pellets and used in our laser vaporization synthesis process [carbon 42, 2004]. The resulting Bio-SWCNT material was thoroughly characterized by Raman, SEM, TG-MS-FTIR, UV-VIS-NIR absorption, and electrical conductivity measurements. All data indicates that the Bio-SWCNT is composed predominantly of nanotubes with relatively little amorphous or impurity carbon content. NIR absorption analysis, in particular, shows a very high intensity of the S22 interband absorption peak, with a NIR absorption purity index [itkis] of 0.185; larger than any we have observed in the literature for as-produced SWCNT, and larger than many reported for post-purified materials. We will present full details of the synthesis and characterization of this exceptional quality SWCNT material, as well as our development of a reference material based on Bio-SWCNT. We will also highlight some of the very positive results obtained from using Bio-SWCNT in transparent conductive film and epoxy resin composite applications.

## 14:59-15:16  Contributed Talk 28

### Control of chiral angles of carbon nanotubes with the catalyst

**Krzysztof Koziol**, *University Of Cambridge, United Kingdom* | **Cate Ducati**, *University Of Cambridge, United Kingdom* | **Alan Windle**, *University Of Cambridge, United Kingdom*

One of the biggest, outstanding challenges in the field is the control of carbon nanotube chirality. The properties of nanotubes, in particular, axial electrical conduction, are highly dependent on chirality, and range from metallic to semiconducting as a function of chiral angle. The industrial applications and future success of the material will rely on controlled synthesis of particular chirality nanotubes. Strategies for sorting nanotubes by chirality look promising (1), although the ultimate objective must be to make exactly the right type of nanotube directly at the synthesis stage. Preferred ranges of chiral angle sometimes invoke crystallographic control from the catalyst. A salient example of chirality selection, if not full control, is provided by multiwall nanotubes grown from an iron carbide catalyst. Strikingly, these show the same chiral angle for each of the nanotube walls, with a strong predisposition to arm-chair and zig-zag structures (2,3). This report explains why such a unique type of nanotube should form, and points to future strategies for the synthesis of nanotubes with special chiralities.  (1) M. Arnold, A. Green, J. Hulvat, S. Stupp, M. Hersam, Nature Nanotechnology 1, 60 (2006). (2) K. Koziol, M. Shaffer, A. Windle, Advanced Materials 17, 760 (2005). (3) C. Ducati, K. Koziol, S. Friedrichs, T. Yates, M. Shaffer, P. Midgley, A. Windle, Small 2, 774 (2006).

## 15:16-15:33  Contributed Talk 29

### Controlled Growth of Single-Walled Carbon Nanotubes on Surface with Desired Structures

**Jin Zhang**, *Center of Nanochemistry, College of Chemistry and Molecular Engineering, Peking University, China*

Due to their excellent properties, single-walled carbon nanotubes (SWNTs) have been regarded as one of the most potential materials for future applications in nanoelectronic devices. However, there is a huge gulf between production and applications. To meet the needs for applications, SWNTs¡¯ diamemter, chirality, metallic/ semiconducting property and architectures should be controlled in the growth process. We present herein a brief review on the growth of SWNTs on surface with controlled structures in our group, including 1) Temperature mediated chemical vapor deposition (CVD) growth of SWNTs with controlled diameter; 2) Cap engineering for SWNTs growth with controlled chirality; 3) Reaction activity diversity induced growth of semiconducting SWNTs; and 4) Combination of two growth modes for fabricating SWNTs on surface with controlled architectures.  Reference  1. Y. G. Yao, Q. W. Li, J. Zhang, R Liu, L.Y. Jiao, Y. Tian, T, Zhu, and Z. F. Liu, Nat. Mater. 6, 283, (2007). 2. Y. G. Yao, C. Q. Feng, J. Zhang, and Z. F. Liu, Nano Lett. 9, 1673 (2009). 3. G. Hong, B. Zhang, B. H. Peng, J. Zhang, W. M. Choi, J. Y. Choi, J. M. Kim, and Z. F. Liu, J. Am. Chem. Soc. 131, 14642, (2009) 4. Y. G. Yao, X. C. Dai, C. Q. Feng, J. Zhang, X. L. Liang, L. Ding, W. Choi, J. Y. Choi, J. M. Kim, and Z. F. Liu, Adv. Mater. 21, 4158, (2009).

## 15:30-16:00  Refreshment Break

## 15:33-17:00 Poster Session 5

**See pages 129-144**

**SESSION CHAIR: A. T. CHARLIE JOHNSON**, *University of Pennsylvania*

## 17:00-17:25 Invited Talk 7

### Towards the nanotube cell phone: digital and FM demodulation in a doubly clamped CNT-NEMS

**Anthony Ayari**, *LPMCN, Université Lyon1 / CNRS, France* | **Thomas Barois**, *LPMCN, Université Lyon1 / CNRS, France* | **Pascal Vincent**, *LPMCN, Université Lyon1 / CNRS, France* | **Vincent Gouttenoire**, *LPMCN, Université Lyon1 / CNRS, France* | **Sorin Perisanu**, *LPMCN, Université Lyon1 / CNRS, France* | **Jean-Louis Leclerc**, *INL, UMR5270 / CNRS Ecole Centrale de Lyon* | **Stephen Purcell** , *LPMCN, Université Lyon1 / CNRS, France*

Carbon Nanotubes (CNTs) have recently been attracting sustained attention as resonators in nanoelectromechanical systems (NEMS). The extremely small physical dimensions of these nanostructures imply high sensitivity to external perturbations and this opens perspectives for novel ultrasensitive, high speed and low power devices in the MHz and GHz range, as well as original experiments in fundamental physics. We present here our recent research on the "nanoradio" concept [1,2]. The Zettl group demonstrated a nanoradio for individual nanotubes in a field emission experiment where the nanotube is attached at one end to a support (singly clamped) [1] and the mechanical resonator acts as a tunable demodulator. In our experiment the CNT resonators are suspended, doubly-clamped, single wall, CNT transistors. This geometry is more amenable to integration as it does not depend on the field emission current which is often unstable. AM, FM and digital demodulation of such devices in the high MHz range for these devices will be shown as well as an identification of the electrical origin of demodulation. The FM technique suppresses unwanted background signals and reduces noise for the detection of mechanical motion of nanotubes. The digital data transfer rate of standard cell phone technology is within reach of our devices [3]. [1] K. Jensen, J. Weldon, H. Garcia, and A. Zettl, Nanoletters 7, 3508 (2007). [2] Rutherglen, C.; Burke, P. Nano Lett. 2007, 11, 3296. [3] V. Gouttenoire, T. Barois, S. Perisanu, J.-L. Leclerc, S.T. Purcell, P. Vincent and A. Ayari, (Small, to be published 2010).

## 17:25-17:42 Contributed Talk 30

### Applications of Aligned Carbon Nanotube Wafer

**Takeo Yamada**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Yuhei Hayamizu**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Yuki Yamamoto**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Yoshiki Yomogida**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Ali Izadi-Nahafabadi**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Don Futaba**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Kenji Hata**, *National Institute Of Advanced Industrial Science And Technology (AIST), Japan*

Motivated to realize reproducible, uniform, and reliable carbon nanotube (CNT) based devices, we developed an approach centered on the use of aligned and closely-packed CNT films, called "CNT wafers" [1]. Through this approach an assembly of a predetermined, massive quantity of aligned CNTs, grown by the super-grown method [2], could be placed at prescribed locations and orientations on silicon substrates, which then could be controllably fabricated into well designed confusions. In this way, functional components with higher structural diversity and complexity could be fabricated and serve as building blocks for device systems. This presentation will contain advances in CNT wafer technology which moved beyond the limitation of silicon substrates to arbitrary surfaces. From the varied structure of the CNT waters, we observed both ductile and brittle mechanical properties, which opened an opportunity to make fully-stretchable devices (i.e. all device components are stretchable). As an example, we fabricated CNT-based strain sensor which showed great performance in range (detect over 250% strain) and cyclic life (over 100,000 cycles), particularly when compared to conventional metal-based strain sensors (detect 5% strain). Because of the wide performance range, we applied this toward the sensing of human motion, an application only possible by few methods. [1] Y. Hayamizu, T. Yamada, K. Mizuno, R.B. Davis, D.N. Futaba, M. Yumura, and K. Hata, Nature Nanotech. 3, 289 (2008). [2] K. Hata, D.N. Futaba, K. Mizuno, T. Namai, M. Yumura, and S. Iijima, Science 306, 1362 (2004).

## 17:42-17:59 Contributed Talk 31

### Enhanced electromodulation of infrared transmittance in semitransparent films of large diameter semiconducting single-walled carbon nanotubes

**Mikhail E. Itkis**, *University of California, Riverside* | **Feihu Wang**, *University of California, Riverside* | **Robert C.Haddon**, *University of California, Riverside*

We study an electro-optical effect in single-walled carbon nanotube (SWNT) thin films in solid state field-effect transistor configuration.(1) We observed an order of magnitude increase of the amplitude of electromodulation of infrared transmission with increasing SWNT diameter from 0.8 to 1.55 nm corresponding to the decrease of the SWNT bandgap from ~1.2 to 0.66 eV. The electromodulated spectral peak is shifted towards the low energy relative to the SWNT absorption peak and the shift increases with decreasing SWNT bandgap reaching a value of 0.4eV in small diameter SWNTs. The nature of this red shift will be discussed. We also observed a superlinear increase of the amplitude of the electromodulation with increasing content of semiconducting SWNTs. The largest amplitude of the effect was observed in large diameter (1.55nm) 99% semiconducting SWNTs and exceeds by more than order of magnitude the results previously reported for SWNT thin film solid state devices. The development of an optical modulator (1) builds on our previous reports of a SWNT infrared bolometer (2) and a SWNT optocoupler,(3) and taken together these studies emphasize the potential of SWNT thin film-based optoelectronics. 1. F. Wang, M.E.Itkis, R.C.Haddon, Nano Letters 10, 937 (2010) 2. M.E.Itkis, F.Borondics, A.Yu, R.C.Haddon, Science 312, 413 (2006) 3. M.E.Itkis, F.Borondics, A.Yu, R.C.Haddon, Nano Letters 8, 2224 (2008) Supported by DMEA

## 17:59-18:16 Contributed Talk 32

### Carbon Nanotube Nanoelectronics and Macroelectronics

**Chongwu Zhou**, *University Of Southern California, USA*

Carbon nanotubes offer great promise but also face significant challenges for future electronic applications. This talk will focus on our recent work on: 1. Assembly and integration of massive aligned nanotubes for nanoelectronics, 2. Metal tube removal based on light irradiation, and 3. Thin film transistors (TFTs) based on separated nanotubes for macroelectronics. We will report our wafer-scale processing of aligned nanotube electronics. Massive aligned nanotubes were synthesized over complete 4 inch quartz and sapphire substrates, and then transferred to Si/SiO2 substrates. CMOS analogous fabrication was performed to yield submicron high performance transistors and defect-tolerant logic circuits. In addition, we will present the metal-to-semiconductor conversion of carbon nanotubes induced by light irradiation. The light irradiation process is scalable to wafer-size scales and capable of yielding improvements in the channel-current on/off ratio up to 5 orders of magnitude in nanotube-based field-effect transistors. Furthermore, we will report wafer-scale processing of TFTs based on separated nanotube, including key technology components such as assembly of high-density, uniform separated nanotube networks, high-yield fabrication of devices with superior performance, and demonstration of organic light-emitting diode (OLED) control circuit. [1] "CMOS-analogous wafer-scale nanotube-on-insulator approach for submicron devices and integrated circuits using aligned nanotubes", Chongwu Zhou et al., Nano Letters, Vol. 9, 189, 2009. [2] "Scalable Light-Induced Metal to Semiconductor Conversion of Carbon Nanotubes", Chongwu Zhou et al., Nano Letters, Vol. 9, 3592, 2009. [3] "Wafer-Scale Fabrication of Separated Carbon Nanotube Thin-Film Transistors for Display Applications", Chongwu Zhou et al., Nano Letters, Vol. 9, 4285, 2009.

# Friday, July 2

**SESSION CHAIR: FEI WEI,** *Beijing Key Laboratory of Green Chemical*

## 8:30-9:10 Keynote 5

### Controlled Growth and Functionalization of Aligned Carbon Nanotubes for Multifunctional Applications

**Liming Dai**, *Department of Chemical Engineering, Case School of Engineering, Case Western Reserve University, USA*

We have previously developed simple pyrolytic methods for large-scale production of vertically-aligned carbon nanotube arrays. The resultant aligned carbon nanotube arrays can be transferred onto various substrates of particular interest in either a patterned or non-patterned fashion. The well-aligned structure provides additional advantages for not only an efficient device construction but also controlled surface functionalization. The controlled surface functionalization of aligned carbon nanotubes is particularly attractive, as it allows surface characteristics of the aligned carbon nanotubes to be tuned in a region-specific fashion while their alignment structure can be largely retained. We have also reported the preferential synthesis of semiconducting vertically-aligned single-walled carbon nanotubes for direct use in FETs even without any purification/separation. Recently, we have further demonstrated that metal-free, nitrogen-doped aligned carbon nanotubes exhibited a high electrocatalytic activity (~4 times of that of the platinum catalyst) for the oxygen reduction reaction (ORR) with an excellent long-term operation stability and free from the crossover/CO-poisoning effect, and that hierarchically-structured aligned carbon nanotube arrays with a straight body segment and a curly entangled top showed almost ten-times stronger shear adhesion force than that of a real gecko foot but still can be easily lifted off in the normal direction when desire. While there is currently a large effort worldwide in developing nanocomposites from nonaligned carbon nanotubes and polymers, the combination of aligned carbon nanotubes with appropriate macromolecules or other materials (e.g., DNA chains, proteins, metal nanoparticles) has also been demonstrated to create synergetic effects, that provide the basis for the development of numerous multifunctional nanocomposite materials and devices, including sensors, membranes, flexible electronics, and energy-related systems. In this talk, I will summarize some of our rational concepts for the controlled growth and functionalization of aligned carbon nanotubes for multifunctional materials and device applications, along with an overview on the recent developments in this exciting field.

## 9:10-9:27 Contributed Talk 33

### Separation of Single Walled Carbon Nanotubes

**Sian Fogden**, *Imperial College, United Kingdom* | **Milo Shaffer**, *Imperial College, United Kingdom* | **Christopher Howard**, *University College London* | **Neal Skipper**, *University College London*

The extraordinary electronic and optical properties of single walled carbon nanotubes (SWNTs) are determined by their structure; SWNTs are either metallic or semiconducting depending on their diameter and chirality(1). Many valuable applications in, for example, transparent conductors, solar cells, biosensors and nanoelectronics, require nanotubes of specific electronic character(2). Current techniques for the separation of SWNTs into semiconducting and metallic species are only partially successful due to the difficulty in the dispersion of SWNTs(3) and separation occurs only on a limited scalability. Here we propose a new, fully scalable method of SWNT separation based on the different susceptibilities of metallic and semiconducting SWNTs to chemical reduction. The method involves SWNT dissolution in metal ammonia solutions where we demonstrate, using small angle neutron scattering data, that these solutions consist of high concentrations of isolated SWNTs. Transferral of these reduced tubes as a dry powder to an organic solvent allows for the spontaneous dissolution of the most easily reduced fraction. Raman scattering and UV/Vis spectroscopy show that this fraction is found to contain predominantly metallic SWNTs. Hence, using this method, metallic SWNTs can easily, quickly and scalably be separated from semiconducting SWNTs. References (1) M. Dresselhaus, G. Dresselhaus, R. Saito, A. Jorio, Physics Reports-Review Section of Physics Letters. 2005, 409, 49. (2) M. Arnold, A. Green, J. Hulvat, S. Stupp, M. Hersam, Nature Nanotechnology. 2006, 1, 60. (3) J. Bahr, E. Mickelson, M. Bronikowski, R. Smalley, Chemical Communications. 2001, 2, 193.

## 9:27-9:44 Contributed Talk 34

### Scalable Structure Separation of Single-Wall Carbon Nanotubes by Multicolumn Gel Chromatography

**Huaping Liu**, *Nanotechnology Research Institute, National Institute Of Advanced Industrial Science And Technology (AIST), Japan; Japan Science and Technology Agency, CREST, Japan* | **Shunjiro Fujii**, *Nanotechnology Research Institute, National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Takeshi Tanaka**, *Nanotechnology Research Institute, National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Ye Feng**, *Nanotechnology Research Institute, National Institute Of Advanced Industrial Science And Technology (AIST), Japan; Japan Science and Technology Agency, CREST, Japan; Institute of Materials Science, University of Tsukuba, Japan* | **Daisuke Nishide**, *Nanotechnology Research Institute, National Institute Of Advanced Industrial Science And Technology (AIST), Japan* | **Hiromichi Kataura**, *Nanotechnology Research Institute, National Institute Of Advanced Industrial Science And Technology (AIST), Japan; Japan Science and Technology Agency, CREST, Japan*

The structural heterogeneity of as-grown single-wall carbon nanotubes (SWCNTs) prevents their widespread application. Recently, our research group developed simple methods for large-scale separation of metallic (M)- and semiconducting (S)-SWCNTs using agarose gel. For the electronic device applications, however, diameter separation of S-SWCNT is also very important for controlling their energy gaps. In this presentation, we report a novel method for the separation of SWCNTs based on multicolumn gel chromatography (MUGEC). By this MUGEC method, not only M- and S-SWCNT separation but also structure separation of S-SWCNTs has been performed. In this novel method, columns were connected end to end and each column was filled with an appropriate amount of Sephacryl gel. SWCNT dispersion was over-loaded onto the first column. M-SWCNTs were eluted with sodium dodecyl sulfate solution from the bottom column. Subsequently, we collected S-SWCNTs from each column by adding sodium deoxycholate solution. S-SWCNT fractions collected from each column show different chirality-enrichments. Especially, from a HiPco SWCNT (diameter, 1.0„b0.3 nm), about 90% pure single chirality of (6, 5) was collected from the first gel column and the other chiralities enriched S-SWCNTs such as (7, 6) and (11, 3) were simultaneously collected from the following columns within 10 minutes. Detailed analysis suggests that MUGEC method can effectively sort S-SWCNTs based on their local curvature radius. This method is simple, quick, high-efficiency, continuous and low cost. Structure separation of S-SWCNTs in industrial scale is expected. We believe that this large-scale structure separation will open a new research field and applications of SWCNTs.

## 9:44-10:01 Contributed Talk 35

### Interactions of Conjugated Polymers with Single-Walled Carbon Nanotubes

**Alex Adronov**, *McMaster University, Canada* | **Patigul Imin**, *McMaster University, Canada* | **Nicole Rice**, *McMaster University, Canada* | **Mokhtar Imit**, *McMaster University, Canada*

Supramolecular functionalization of carbon nanotubes with conjugated polymers is particularly attractive due to the versatility of polymer structures, both in terms of backbone and side chains, which allows the preparation of polymer-nanotube complexes that exhibit a wide variety of interesting and useful properties. This includes control over polymer bandgap and electron affinity, enabling the modification of optoelectronic properties of the polymer-nanotube conjugate. In addition, varying polymer side-chains can modify the solubility and electrostatic nature of the polymer. This not only allows for modification of compatible solvents for the polymer-nanotube complexes, but also enables electrostatic patterning (including layer-by-layer deposition) and electrophoretic deposition of carbon nanotubes on various surfaces. We have shown that a variety of tailor-made conjugated polymers can form extremely strong pi-stacking interactions with the surface of carbon nanotubes, and the properties of the resulting polymer-nanotube complexes are strongly dependent on the polymer backbone structure, the nature of the side-chains, and the polymer molecular weight. This presentation will highlight the preparation, characterization, and applications of complexes between new conjugated polymers and carbon nanotubes.

## 10:00-10:30 Coffee Break

## 10:01-11:30 Poster Session 6

**See pages 145-161**

**SESSION CHAIR: MARIANNA FOLDVARI**, *University of Waterloo*

## 11:30-11:55 Invited Talk 8

### Development of Multiwalled Carbon Nanotubes for Cancer Therapy

**Andrew Burke**, *Department of Cancer Biology* | **Ravi Singh**, *Department of Cancer Biology* | **David L. Carroll**, *Department of Physics; Comprehensive Cancer Center, Wake Forest University School of Medicine* | **John Owen**, *Section of Hematology/Oncology* **Roy Hantgan**, *Department of Biochemistry* | **Frank M. Torti**, *Department of Cancer Biology; Comprehensive Cancer Center, Wake Forest University School of Medicine* | **Suzy V. Torti**, *Department of Biochemistry; Comprehensive Cancer Center, Wake Forest University School of Medicine, USA*

The emergent properties of nano-scale multiwalled carbon nanotubes (MWCNTs) render them an ideal platform for the development of multifunctional agents for the treatment of cancer. We have recently demonstrated that pluronic-coated MWCNTs are biocompatible and efficiently mediate the thermal destruction of cancer cells in vitro and tumor xenografts in vivo when used in conjunction with near-infrared laser radiation (1). Encouragingly, the rapid thermal ablation of tumors achieved using this technique translated into long-term survival for treated animals with no evident systemic toxicities. Further development of nanotubes as therapeutic agents will likely involve intravenous delivery. This requires that carbon nanotubes demonstrate compatibility with normal circulatory components, including cellular blood constituents and proteins of the hemostatic cascades. In the present study, we investigated the role of nanotube coating and functionalization on interactions with blood components. We observed that nanotube preparations activate the intrinsic coagulation cascade through novel and specific interactions with coagulation factors. In addition, nanotubes activated platelets in vitro in a manner dependent on coating and functionalization. Coating and functionalization also exerted profound effects on the ability of nanotubes to activate platelets in mice. These findings will inform the development of multiwalled nanotubes as biocompatible nanomaterials for systemic delivery, an essential step in the translation of these research materials into validated clinical tools. 1. Burke, A., et al. (2009) Long-Term Survival Following a Single Treatment of Kidney Tumors with Multiwalled Carbon Nanotubes and near-Infrared Radiation Proc Natl Acad Sci USA 106, 12897-12902.

## 11:55-12:12 Contributed Talk 36

### Anabolic steroids recognition with carbon nanotubes field-effect transistor arrays

**M. Teresa Martinez**, *Instituto De Carboquímica CSIC, Spain; Molecular Foundry, LBNL, USA* | **Yu-Chih Tseng**, *Department of Electrical Engineering and Computer Sciences, University of California at Berkeley, USA* | **Juan Pablo Salvador**, *Applied Molecular Receptors Group (AMRg), Chemical and Biomolecular Nanotechnology Department,Spain; Networking Research Center on Bioengineering, Biomaterials and Nanomedicine, CIBER-BBN* | **Pilar Marco**, *Applied Molecular Receptors Group (AMRg), Chemical and Biomolecular Nanotechnology Department,Spain; Networking Research Center on Bioengineering, Biomaterials and Nanomedicine, CIBER-BBN* | **Nerea Ormategui**, *CIDETEC Pº Miramón, Spain* | **Iraida Loinaz**, *CIDETEC Pº Miramón, Spain* | **Jeffrey Bokor**, *Department of Electrical Engineering and Computer Sciences, University of California at Berkeley, USA; Molecular Foundry, LBNL, USA*

A proof of concept of the electronic detection of two anabolic steroids, Stanozolol (Stz) and Methylboldenone, (MB), was carried out using two specific antibodies and arrays of carbon nanotube field effect transistors (CNTFETs). Antibodies specific for Stz, and MB, were prepared and immobilized on the carbon nanotubes (CNTs) using two different approaches; direct non-covalent bonding of antibodies to the devices, and bonding the antibodies covalently to a polymer that had been previously used for the DNA hybridization detection (1). The results indicated that CNTFETs bonded to specific antibodies covalently or non-covalently are able to detect the presence of steroids. Statistically-significant changes in the threshold voltage and drain current were registered in the transistors, allowing the steroids to be recognized (2). On the other hand, it was determined that the specific antibodies do not detect other steroids other than Stz and MB, such as Nandrolone (ND). Regarding the detection mechanism, in addition of charge transfer, Schottky barrier, SB, modification and scattering potential reported by other authors, electron/hole trapping mechanism leading to hysteresis modification has been determined. The presence of polymer hinders the modulation of the electrode-CNT contact. 1.- Martínez, M. T.; Tseng, Y-C.; Ormategui, N.; Loinaz, I.; Eritja, R.; Bokor. Label-Free DNA Biosensors Based on Functionalized Carbon Nanotube Field Effect Transistors .. Nano Lett. , 2009, 530-536. 2.- MT Martínez, Y. C. Tseng , J.P. Salvador, MP Marco, N. Ormategui , I. Loinaz ,J. Bokor Electronic anabolic steroids recognition with carbon nanotubes field effect transistors ACSnano (on line http://pubs.acs.org/journal/ 08.02.2010)

## 12:12-12:29 Contributed Talk 37

### A comparative study of the potential impact of DWNT on human health and the environment

**Emmanuel Flahaut**, *CIRIMAT-CNRS ; Institut Carnot Cirimat, France* | **Bernard Pipy**, *EA 2405 - Université Paul Sabatier Toulouse III IFR 31 Institut Louis Bugnard, France* | **Ludovic De Gabory**, *Inserm U577, University Bordeaux II, France* | **Laurence Bordenave**, *Inserm U577, University Bordeaux II, France* | **Florence Mouchet**, *Université de Toulouse; UPS, INP; EcoLab ; ENSAT, France* | **Laury Gauthier**, *Université de Toulouse; UPS, INP; EcoLab ; ENSAT, France*

Carbon nanotubes (CNT), with an annual world production reaching several hundreds of tons, represent a special category of nanomaterials with exceptional characteristics and numerous potential applications. Although the toxicity and the environmental impact of CNT have now both been investigated by different groups (although the latter never focused much attention until very recently), there is yet a controversy about the results and still no answer to the simple question: 'are CNT toxic?' The fact is that the large range of kinds of CNT and methods to produce and then (in most cases) process them make any comparison almost impossible. The results presented here have been obtained with the same batch of CCVD-produced DWNT [1] and concern both the investigation of their potential impact on human health (in vitro models) and the environment (in vivo models) [2]. They lead to the conclusion that all the experimental parameters (dealing both with CNT and biological models used) play a very important role and can easily explain the large differences between the results obtained by the different researchers. The main conclusions of our studies will be presented. References: [1] E. Flahaut et al., Chem. Comm. (2003) 1442. [2] F. Mouchet et al., Env. Toxicology, (2009), in the press.

**SESSION CHAIR: CHRIS KINGSTON**, *National Research Council Canada*

## 14:00-14:25 Invited Talk 9

### Exploring functionalized carbon nanotubes for cancer therapy

**Alberto Bianco**, *CNRS - Centre National De La Recherche Scientifique, France*

The applications of carbon nanomaterials, and particularly carbon nanotubes (CNTs), in the emerging field of cancer therapy are intensifying (A. Bianco et al. Expt. Opin. Drug Deliv. 2008, 5, 331; K. Kostarelos Nature Nanotech. 2009, 4, 627). CNTs hold a lot of promises for biomedical applications for different reasons: they are highly stable, water dispersible/soluble, non immunogenic, efficiently loaded with therapeutic molecules, and rapidly internalized into cells (K. Kostarelos et al. Nature Nanotech. 2007, 2, 108). The organic functionalization has facilitated the manipulation of this type of nanomaterials, thus opening the way to the potential use of CNTs as novel tools for drug delivery (D. Tasis et al. Chem. Rev. 2006, 106, 1105). Functionalized CNTs can be considered as a promising alternative to the common drug delivery systems. In this context, we have explored the possibility of targeted delivery of small organic molecules (antibiotics and anticancer agents), bioactive peptides and nucleic acids (M. Prato et al. Acc. Chem. Res. 2008, 41, 60). In this presentation we will describe the functionalization of CNTs with small drugs (Samorì et al. Chem. Commun. 2010, 46, 1194) and siRNA for applications in cancer therapy. Advantages of CNTs in therapeutic silencing in vivo over other delivery systems will be presented (J. E. Podesta et al. Small, 2009, 5, 1176). We will also address the critical issue of CNT toxicity (L. Lacerda et al. Adv. Mater. 2008, 20, 225).

## 14:25-14:42 Contributed Talk 38

### Separation of metallic and semiconducting carbon nanotubes by matrix-free vertical electrophoresis with nonionic surfactant

**Kazuki Ihara**, *Nanotube Research Center, National Institute of Advanced Industrial | Science and Technology (AIST), Japan* **Takeshi Saito**, *Nanotube Research Center, National Institute of Advanced Industrial | Science and Technology (AIST), Japan* | **Hiroyuki Endoh**, *Nano Electronics Res. Labs., NEC Corp., Japan* | **Fumiyuki Nihey**, *Nanotube Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Japan*

Electrophoresis is a high-yield, low-cost, and scalable method for the separation of metallic and semiconducting single walled carbon nanotubes (SWCNTs). However, almost all reports used ionic surfactants, which must be removed for further electronic applications such as thin-film transistors. We achieved a distinct separation of metallic and semiconducting single walled carbon nanotube (SWCNT) by using matrix-free vertical electrophoresis with nonionic surfactant. The apparatus for the electrophoresis was consisted of a vertical cell with a cathode and an anode located at the top and bottom, respectively. As-produced SWCNTs with an average diameter of 1 nm were dispersed into deuterium oxide with nonionic surfactant of polyoxyethylene stearyl ether (Brij 700, Aldrich) by using ultrasonic and ultracentrifuge. Separation was carried out by applying DC voltage for the dispersion filled in the cell without supporting matrix. After 16 hours, two colored layers were separately formed at the both side of cell (red and blue for the upper and lower side, respectively). UV-vis-NIR absorption spectroscopy showed that metallic SWCNTs were enriched in the upper layer whereas semiconducting were enriched in the lower. The concentration of semiconducting SWCNT exceeded 95% for the bottom layer. We also found that this method can be applied for the SWCNT with a wide range of diameters (1-2 nm), and even for the dispersion without centrifuge treatment.

## 14:42-14:59 Contributed Talk 40

### One step towards characterization of chirality distribution by the analysis of background extinction in optical absorption spectra of SWCNTs

**Takeshi Saito**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan* | **Shigekazu Ohmori**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan* | **Masayoshi Tange**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan* | **Bikau Shukla**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan* | **Toshiya Okazaki**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan* | **Motoo Yumura**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan* | **Sumio Iijima**, *National Institute of Advanced Industrial Science and Technology (AIST), Japan*

For precise characterizations of SWCNTs by optical absorption spectroscopy, the background extinction originated from precipitable impurities and SWCNTs' bundles has been experimentally determined by interval centrifugation and difference spectrum (IC-DS) technique. The baseline correction using the lineshape of obtained background extinction revealed the actual absorption spectrum of absolutely de-bundled SWCNTs with detailed features. Deconvolution of the corrected absorption spectrum into multiple Lorentzian lines enables the evaluation of chirality distribution including both semiconducting and metallic SWCNTs in the diameter range wider than that feasible by a general photoluminescence (PL) spectroscopy. More interestingly, the resulted chirality distribution of semiconducting SWCNTs was confirmed to be well consistent with the result of PL mapping measurements. Hence this method of characterizing chirality distribution with IC-DS technique has been appeared to be useful as a complement to the PL mapping analysis. This work has been partially supported by New Energy and Industrial Technology Development Organization (NEDO) project.

## 14:59-15:16 Invited Talk 10

### Recent Progress in Carbon Nanotube Sorting by DNA

**Ming Zheng**, *National Institute Of Standards And Technology, USA*

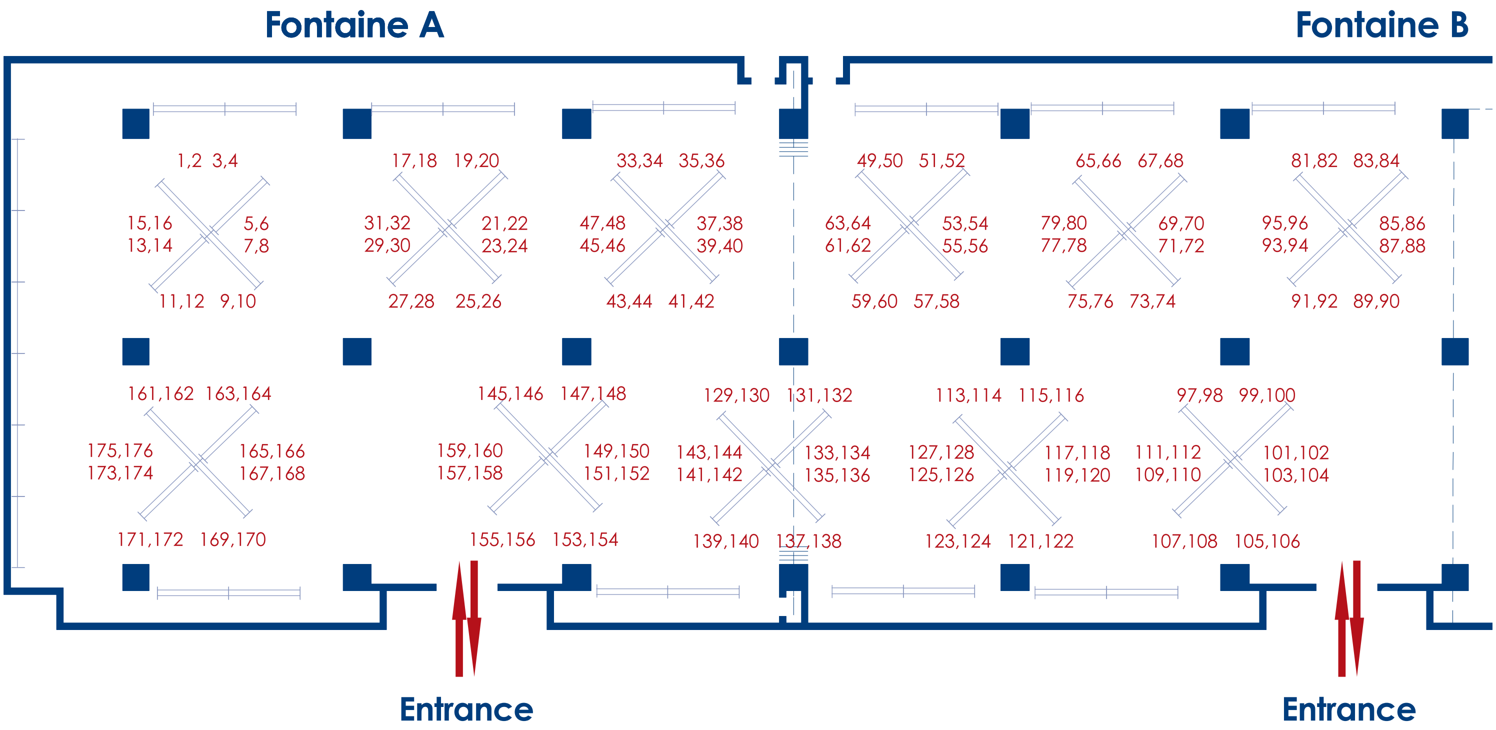
Single wall carbon nanotubes (SWCNT) are a family of molecules that have the same cylindrical shape but different chiralities. The SWCNT sorting problem, i.e., separation of a synthetic mixture of tubes into individual single-chirality components, has attracted considerable attention in recent years. A systematic and general method to purify each and every single-chirality species of the same electronic type from the synthetic mixture is highly desirable. Recently, we have reported such a method that allows purification of all 12 major single-chirality semiconducting species from a synthetic mixture, with sufficient yield for both fundamental studies and application development (Tu et al., Nature, 406, 250, 2009). In this presentation, I will review the experimental development and mechanistic understanding of the separation process. In particular, a model of DNA wrapping structure invoking a novel secondary DNA structure motif will be discussed.

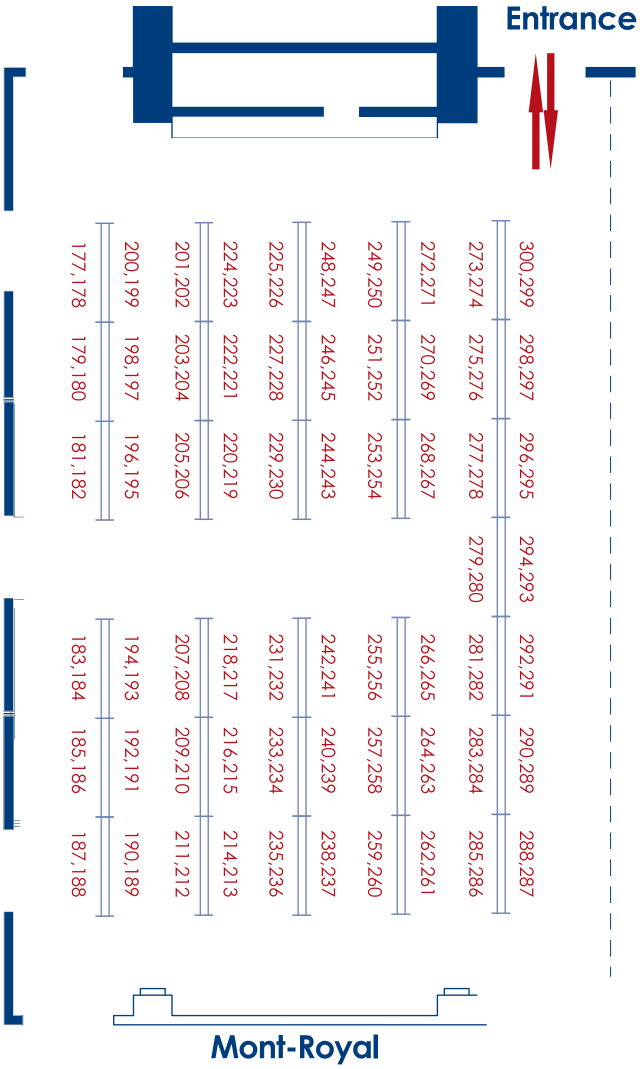
## 15:16-16:00 Summary

**Mildred Dresselhaus**, *Department of Electrical Engineering & Computer Science and Department of Physics, MIT, USA*

## 16:00 Closing Remarks

# Poster Session Floor Plan





# Poster Sessions

## ROOM: FONTAINE AB & MONT-ROYAL

## Tuesday, June 29

### 7:00-8:30 Poster set-up (for Poster Sessions 1-3)

### 10:01-11:30 Poster Session 1

### Poster Board | 1

#### Doping dependence of the Raman intensity of graphene close to the Dirac point

**Cinzia Casiraghi**, *Freie Universität Berlin, Germany*

Raman spectroscopy is a fast and non-destructive means to characterize graphene. Doping strongly affects the G and 2D peaks shape and intensity [1-2]. In particular, the 2D intensity is strongly affected by the electron-electron scattering rate, which increases with doping [3]. Here we use the 2D peak intensity variation with doping to extract the electron-phonon scattering rate [3]. We use pristine and non-gated graphene samples, where the Fermi level shift is induced by charged impurities, in order to probe the 2D peak dependence much closer to the Dirac point than in gated graphene samples [4-5]. We find an electron-phonon scattering rate of 60 ps-1, measured at 2.41 eV [5]. 1. S. Pisana et al, Nature Mat. 6, 198 (2007) 2. A. Das et al., Nature Nanotech. 3, 210 (2008) 3. D. M. Basko et al. PRB 80, 165413 (2009) 4. C. Casiraghi et al., APL 91, 233108 (2007) 5. C. Casiraghi, PRB 80, 233407 (2009)

### Poster Board | 4

#### Investigation of the graphene / 6H-SiC(000-1) interface using scanning tunneling microscopy and ab initio calculations

**Fanny Hiebel**, *Institut Neel CNRS-UJF, France* | **Pierre Mallet**, *Institut Neel CNRS-UJF, France* | **Laurence Magaud**, *Institut Neel CNRS-UJF, France* | **Jean-Yves Veuillen**, *Institut Neel CNRS-UJF, France*

Graphitization of the polar faces of SiC can provide macroscopic graphene films. However, possible interaction with the substrate has to be investigated. The graphene / SiC(0001) (Si face) interface is well characterized. The first graphitic plane strongly interacts with the substrate and acts as a « buffer layer ». Therefore, the graphene electronic structure only shows up for the second graphitic plane. Graphene films grown on the SiC(000-1) (C face) show better transport characteristics. Because of charge transfer from the substrate, the interface plays an important role in such experiments but largely remains to be characterized. We prepared lightly graphitized C face samples under ultra-high vacuum (Hiebel et al., Phys. Rev. B 78, 153412 (2008)). They exhibit monolayer graphene islands with various orientations. Under the islands, we identify two interface structures, namely the native C face reconstructions labeled (3x3) and (2x2)C. We analyze the local density of states (at low energy) for each type of island (G_3x3 and G_2x2). On the G_3x3 islands, we observe a uniform honeycomb structure, indicating a very small substrate interaction. On the G_2x2 islands, the honeycomb structure is slightly, periodically perturbed. Further investigation of the G_2x2 structure using ab initio DFT calculations reveals a small interaction that only affects the graphene electronic structure for energies about 0.5 eV above the Dirac point (Magaud et al., Phys. Rev. B 79, 161405 (2009)). Thus, at variance with the Si face, the C face is efficiently passivated by its surface reconstructions.

### Poster Board | 7

#### Analytical Study of Optical Absorption in Single-Wall Carbon Nanotubes

**Abbas Zarifi**, *Yasouj University, Iran*

Optical absorption in carbon nanotubes strongly depends on the polarization direction of the incident light. Optical properties in carbon nanotubes for light polarized parallel to the nanotube axis have been investigated semianalytically however for light polarized perpendicular to the nanotube axis no calculations have been reported so far. We propose a method to be able to obtain the electric dipole matrix in carbon nanotubes for perpendicular polarization and then by virtue of that we investigate the optical properties in carbon nanotubes semianalytically. We focus on the optical absorption spectra of electrons for carbon nanotubes with arbitrary chirality for light polarized perpendicular to the nanotube axis, semianalytically. We get completely different resonant energy positions for different polarization directions. Further some small resonance peaks below and after the two times the nearest-neighbor overlap integral all carbon nanotubes show a high resonance peak around that value regardless of their chirality. Semiconducting carbon nanotubes moreover show a very high resonance peak associated to the fundamental gap energy. For metallic carbon nanotubes this peak is less pronounced.

### Poster Board | 10

#### Graphene electro-mechanical switch: simulations for reaction barriers and electronic states

**Takazumi Kawai**, *Nano Electronics Res. Labs, NEC Corp., Japan* | **Yoshiyuki Miyamoto**, *Nano Electronics Res. Labs, NEC Corp., Japan* | **Stephan Roche**, *CEA, INAC, SP2M, L_sim, France; CIN2 (CSIC-ICN), campus U.A.B., Spain*

Graphene is one of the most fascinating materials because of its peculiar electronic states due to 2D network of pi electrons, and also because of its robustness against the mechanical deformation and high temperature. Using these properties, graphene based switches are proposed in the experiment [Standley, et al., Nano Lett. 8, 3345 (2008)]. They claimed that several defect structures were formed in the graphitic networks depending on induced current and those defects caused different conductivities. However, the mechanism of atomic-scale switching and its atomic structures are still not clear. In this paper, we propose a mechanism for atomic switch of graphene with Stone-Wales (SW) transformations. Two different structures for the switch consist of two graphene sheets connected with continuous sp2 network or a line of SW defects. Using nudged elastic band method (NEBM) we estimated reaction barriers for the transformation between two different structures under tension. The 10 % tension reduced the barrier height and the stability of the structure with a line of SW defects. The conductivity of the structure with a line of SW defects would be suppressed due to the disconnection of the network of pi electrons. We will discuss the atomic structures and electronic states in detail at the poster.

### Poster Board | 13

#### Electron/hole coexistence in disordered graphene probed by high-field magneto-transport

**Jean-Marie Poumirol**, *LNCMI, Université de Toulouse, France* | **Walter Escoffier**, *LNCMI, Université de Toulouse, France* | **Amit Kumar**, *LNCMI, Université de Toulouse, France* | **Goiran Michel**, *LNCMI, Université de Toulouse, France* | **Raquet Bertrand**, *LNCMI, Université de Toulouse, France*

We report on magneto-transport measurements in disordered graphene under pulsed magnetic field of up to 57T. For large electron or hole doping, the system displays the expected anomalous Integer Quantum Hall Effect (IQHE) specific to graphene. In the close vicinity of the charge neutrality point, the system breaks up into co-existing puddles of holes and electrons, leading to a vanishing Hall resistance. The longitudinal resistance remains finite with no sign of divergence at high magnetic field. Large resistance fluctuations are observed, with maximum amplitude when the magnetic length is comparable with the mean size of the electron-hole puddles.

## Poster Board | 16

### Porphyrin non-covalently functionalized graphene in aqueous suspensions

**Jianxin Geng**, *Korea Advanced Institute Of Science & Technology, Korea* | **Seung-Bo Yang**, *Korea Advanced Institute Of Science & Technology, Korea* | **Hee-Tae Jung**, *Korea Advanced Institute Of Science & Technology, Korea*

Graphene has potential application in techniques such as nanoelectronics, nanocomposites, conductive and transparent films due to its unique structure and physical properties. Synthesis of graphene is one of the major research efforts in order to make rapid developments in graphene research. In this study, a new method, that makes use of the PI-PI interactions between porphyrin and graphene sheets to stabilize the chemically converted graphene (CCG), has been developed for preparation of dispersible CCG via chemical reduction of exfoliated graphene oxide (GO). The porphyrin functionalized CCG suspension can be stable at least for several months. The PI-PI interactions of porphyrin with graphene have been characterized by optical absorption and Raman spectroscopy. In order to demonstrate the advantages of the porphyrin functionalized CCG suspension, conductive graphene films with various thicknesses have been prepared by using the porphyrin functionalized CCG suspension via a vacuum filtration method. It is found that the change of the sheet resistance of the CCG films follows percolation mechanism. With 80 % transparency at 550 nm, the CCG films show sheet resistance as low as ca. 5 Kohms/square. Such low sheet resistance is contributed to improved sp2 networks of the CCG sheets and low contact resistance between the CCG sheets, which is achieved by combination of chemical reduction of GO and thermal annealing of the resultant CCG films.

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### Graphene Oxide-Based Immune-Biosensor for Pathogen Detection

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In this study, we demonstrated a graphene oxide (GO)-based immune-biosensor system for pathogen detection using fluorescence quenching effect between GO and gold nanoparticles. The fluorescent GO sheets was deposited on an amino-modified glass surface by electrostatic force, and the carboxylate functional group on the GO surface was used to covalently conjugate Rotavirus-antibodies to be linked on the surface. The target pathogen, Rotavirus, was then incubated and bound by a specific antigen-antibody interaction. Finally, an engineered gold nanoparticle-labeled antibody probe was attached to the captured target cell which complexes enable gold nanoparticles to be close to the GO surface, thereby resulting in the quenching of GO fluorescence signal to identify the pathogen. This novel GO immuno-biosensor platform provides much cheaper, facile and robust bioassays than the conventional methods.

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### Correlating surface studies with magneto transport measurements on epitaxial graphene.

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Epitaxial graphene can be grown on silicon carbide substrate via the thermal sublimation of the silicon atoms. The graphitization can be obtained under ultra-high vacuum (UHV) conditions or in controlled atmosphere and starting either from the 6H-SiC(0001) (Si face) or from the 6H-SiC(000-1) (C face) surfaces. In order to understand the relationship between growth conditions and the resulting atomic and electronic structure, we have performed scanning probe imaging and low temperature magneto transport studies of graphitized 6H-SiC surfaces obtained in different conditions. Surface morphology is characterized by atomic force and scanning tunnelling microscopy at large and atomic scale respectively. Depending on the intrinsic disorder observed on the samples and on the mobility, the magneto resistance shows either the conventional weak localization or the weak anti localization (WAL) in agreement with the recent WAL theory for graphene [E. McCann et al. PRL 97, 146805 (2006)]. The adjustment of the experimental data gives access to the scattering mechanism corresponding to the different growth conditions.

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### Flexible room-temperature gas sensors based on graphene films

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We present a flexible room temperature gas sensor platform consisting of CVD-grown graphene films or vertical carbon nanotubes (CNTs)/reduced graphene hybrid films supported by polyimide substrates. The CVD-grown graphene films of 3~5 layers showed a highly sensitive and fast response to sub-ppm NO2 gas. A hybrid film, formed by the growth of a vertically aligned CNT array (with CNTs 20 um in length) on the reduced graphene film surface, exhibited relatively slow response with weak N-P transitions. The outstanding flexibility of the graphene-based films ensured stable sensing performances in devices submitted to extreme bending stress. The tunable, large-scale, and reproducible graphene-based films can be readily integrated into the flexible gas sensor devices.

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### Transport Studies through Graphene Bilayer p-n Junction

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Graphene bilayers show promise for future device applications resulting from their theoretically attainable high on/off ratio. In one study, a on/off ratio of 10^3 was achieved by application of a high transverse electric field, which produced a band gap due to the breaking of A and B lattice symmetries[1]. It has also been proposed that the creation of a barrier, as in a p-n junction, impedes the transmission of chiral charge carriers in the case of normal incidence on the barrier[2]. This too will lead to a theoretically high on/off ratio without the need for application of a large electric field. Such p-n junction devices were fabricated using a buried split gate device structure in the 300mm fabrication facilities at UAlbany. Process techniques were developed using current semiconductor industry tools and processes in order to leave a planar 100nm SiO2 surface on top of buried split gates on 300mm Si wafers. Graphene was exfoliated onto the SiO2, and the buried gates used to electrostatically dope the graphene, thus creating a potential step which impedes charge carriers' transmission. Electron beam lithography was used to create source and drain contacts on the respective p and n regions of the graphene. Such devices have the advantage of not needing any permanent dielectric on top of the graphene, and proper annealing leaves large area, pristine bilayers. A detailed study of process conditions, deposition techniques, annealing conditions, Raman analysis, and electrical measurements will be presented. [1]Xia et al. doi: 10.1021/nl9039636 [2]Katsnelson et al. doi: 10.1038/nphys384

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### Carbon nano-flakes produced by ICP thermal plasma system

**Ramona Pristavita**, *McGill University, Canada* | **Jean-Luc Meunier**, *McGill University, Canada* | **Dimitrios Berk**, *McGill University, Canada*

There is presently an effort in the development of hydrogen fuel cells such as PEM fuel cells. Even if the PEM fuel cells are a clean and efficient alternative energy source, production cost must be reduced substantially in order for them to be economically viable. Three components of the PEM fuel cells, namely the electrodes, the membrane and the catalyst account for 80% of the production cost. While the price of the electrodes and membrane is predicted to decrease, the price of the catalyst would remain the same or even increase due to a constant increase in the Pt price. One possible way to reduce this cost is to develop an alternative, low cost catalyst. The proposed material in this project consists of a carbon black powder which contains nitrogen atoms bonded to the graphitic support and iron atoms coordinated to the nitrogen atoms, creating the active centers of the catalyst. The carbon nanopowders were obtained by plasma decomposition, using an ICP system, of methane at various flow rates and show a uniform microstructure throughout the reactor. The obtained product has a crystalline graphitic structure, with a stacking of between 6 and 16 planes and a nano-flake morphology with particles dimensions of approximately 100 nm long, 50 nm wide and 5 nm thick. Nitrogen was also introduced in some synthesis experiments using flow rates of 0.1slpm and 0.2 slpm. The resulting product has the same structural properties and the nitrogen is incorporated into the graphitic structure thought pyridinic type bonds.

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### The Low-Temperature Conduction Anomaly in Graphene

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The resistance R(T) of graphene often shows a monotonic increase or decrease as temperature increases from 4.2 K to around 70 K. We find this anomaly can change sign for even very small changes in gate voltage, indicating that it is not a systematic effect. Using the field effect transistor configuration, we have conclusively determined the cause of this anomaly as arising from the decay of mesoscopic resistance fluctuations (MRFs) due to progressive dephasing of the interfering scattered electron waves as T increases. Our measurements of R(T) at different constant gate voltages Vg tuned to different features of the MRFs observed in R(Vg) at constant temperature reveal some surprising features not well understood by current theory, for example the exponential rather than power law decay of MRFs with temperature, and the variation of MRF properties as Vg changes [1]. [1] V. Skákalová, A.B. Kaiser, J.S.Yoo, D. Obergfell and S. Roth, Phys. Rev. B 74, 153404 (2009).

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### Uniform Graphene Oxide-Phthalocyanine Thin Film Fabricated by Electrostatic Layer-by-Layer Self-Assembly

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As a novel 2D nano-material, graphene has attracted great attentions for its outstanding electronic, optical and mechanical properties. Recently, to endow graphene with optoelectronic properties for promising applications on solar cell and LED, planar aromatic dyes such as porphyrins and phthalocyanines were combined into the design of graphene composites by covalent or non-covalent modifications. However, quite few attempts have been applied to explore approaches for the fabrication of graphene-dye thin films. Herein, we report a simple strategy to obtain graphene oxide-copper phthalocyanine (GO-CuPc) thin film with different thickness by electrostatic layer-by-layer (LbL) self-assembly. AFM, UV-Vis spectroscopic and ellipsometry investigations suggest that the films are highly uniform with well-controlled thickness up to 60nm thick. Furthermore, a detailed spectroscopic ellipsometry evaluation provided accurate refractive indices of the film thickness. This LbL self-assembly method is successfully applied to various substrates, including quartz, ITO glass, silicon and mica. The GO-CuPc films show good stability and high uniformity on the different substrates, which is ideal for potential electronic applications. The thin films show photovoltaic response to visible light. UV-vis spectra and AFM imagines reveal that the the GO-CuPc films can response to acid gas and therefore have potential applications in novel chemical sensors.

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### Graphene Nanoconstriction Field Effect Transistor

**Ye Lu**, *University Of Pennsylvania, USA* | **Brett Goldsmith**, *University Of Pennsylvania, USA* | **Douglas Strachan**, *University Of Kentucky* | **A.T. Charlie Johnson**, *University Of Pennsylvania, USA*

We report an approach to fabricate monolayer graphene nanoconstriction field effect transistors (NCFETs) with critical dimensions below 10 nm, a regime that is not accessible by conventional nanolithography. We start by fabricating a gold nanowire on top of mechanically-exfoliated monolayer graphene. We use Feedback Controlled Electromigration to form a nanoconstriction in the gold wire, which is then used as an etch mask for the graphene during an oxygen plasma patterning step. We observe the opening of a confinement-induced energy gap as the NCFET width is reduced, as evidenced by a sharp increase in the NCEFT on/off ratio, which can be as large as 1100 at room temperature for the thinnest devices. Such devices deliver up to 100microampere current at 50mV bias with an on state resistance of 50kilo ohm, which is at least an order of magnitude lower than graphene nanoribbon FETs with similar on/off ratio. This lower resistance is due to large area contacts in our devices.

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### Studies of graphene monolayers and bilayers by Raman spectroscopy

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Graphene is described as a monolayer of carbon atoms arranged in a two-dimensional honeycomb lattice. One of the most interesting properties of this material is related to its electronic band structure which permits carriers to behave as massless Dirac fermions with vanishing density of states at the Fermi level [1]. If two graphene layers are stacked in Bernal AB configuration these properties are destroyed as the electronic dispersion curve is no more linear but parabolic. However, for a misoriented stacking in graphene bilayer, the dispersion curve reverts back from parabolic to linear as on monolayers [2,3]. The graphene monolayers and bilayers can thus be viewed as two different materials with high interest for both fundamental and applied physics. Raman spectroscopy is a nondestructive and quick technique largely applied to characterize graphene samples. The spectral signature of second order peak (2D) is used to identify graphene monolayers and few layers [4,5]. In this work, we studied by resonant Raman spectroscopy the dependence of 2D frequency and lineshape on the laser excitation energy for monolayers, Bernal bilayers, and misoriented bilayers. The comparison between the Raman response of monolayers and bilayers on different substrates was also investigated. In addition, results obtained on exfoliated graphene ribbons using several laser wavelengths will be presented and compared with the data obtained on large graphene flakes. [1] Novoselov et al., Science 306,666(2004). [2] Latil et al., PRB 76,201402(2007). [3] Poncharal et al., PRB 78,113407(2008). [4] Ferrari et al., PRL 97,187401(2006). [5] Malard et al., Phys.Rep. 473,51(2009).

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### Spin polarization and magnetic phase control of graphite thin films

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Graphene has been extensively paid attentions because of its unique electric property. In particular, electron mobility along the carbon layer is about ten times higher than that of the silicon. This characteristic property is resulting from the topology of the two-dimensional pi electron network and the linear dispersion of the bands at the Fermi level. Besides the perfect two-dimensional graphene sheet, when graphene flaks or ribbons have edges with a zigzag shape, there is another peculiar electronic state at the Fermi level. This state is known as the edge state that is extended along the edge region with certain magnetic ordering: polarized electron spins are ferromagnetically aligned along each edge while antiferromagnetically coupled between two edges. In the present work, based on the first-principle total-energy calculations, we clarify that (0001) surfaces of rhombohedral (ABC stacking) graphite show magnetic ordering at the surface region. The origin of the polarization is the flat-band states at the Fermi level, which is resulting from the edge state similar to the graphene ribbon. We demonstrate the possibility of phase control on magnetic state of rhombohedral graphite layers by applying the external electric field normal to the layer. Our calculations clearly show that the rhombohedral graphite undergoes magnetic phase transition from ferrimagnetic to ferromagnetic states under the moderate electronic field. The present results give the possibility of applications of the graphite thin layers for a constituent material in spintronics devices with MOSFET structure.

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### Nanomachining graphene with irradiation

**Jani Kotakoski**, *University Of Helsinki, Finland* | **Ossi Lehtinen**, *University Of Helsinki, Finland* | **Arkady Krasheninnikov**, *University Of Helsinki, Finland; Aalto University, Finland*

Graphene is the ultimately thin membrane - a chicken wire structure made from sp2-hybridized carbon atoms - which has attracted enormous attraction since its recent discovery, not least because of its unique electronic properties. An important aspect in this regard is the effect of disorder, especially since CVD grown graphene is known to contain a large proportion of dislocations. Ion irradiation is a good method for systematically studying the effect of disorder because the doses and hence disorder can be controlled. Since the atomic level events occurring under ion irradiation of graphene have remained unknown, we have combined DFT and empirical potentials to run dynamical computer simulations to describe these atomic scale events. Also, combining DFT simulations and TEM experiments, we have investigated the processes occurring in graphene under electron microscopy, and explained how the electron beam introduces defects such as bond rotations and vacancies in the structure.

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### Observation of coherent excitation of the interlayer shearing mode in multilayer graphene

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Raman spectroscopy is one of the key methods for the characterization of single and multilayer graphene. In the bulk limit, the lateral motion of adjacent graphene planes gives rise to a Raman active low-frequency mode, the so-called interlayer shearing mode. Coherent excitation of this mode has been observed by femtosecond time-resolved reflectivity [1]. For the case of few-layer graphene, related modes are predicted to be present and to exhibit different properties as a function of layer thickness [2]. Here we report the observation of coherent oscillation of such shearing mode phonons in multilayer graphene. The experiments are performed on mechanically exfoliated graphene samples using femtosecond laser excitation pulses and time-delayed femtosecond probe pulses in a transient reflectivity measurement. We will discuss the characteristics of shearing mode phonons as a function of the thickness of multilayer graphene. The coherent shearing-mode phonons in graphite exhibit a period of 800 fs, with a damping time of around 10 ps. Reducing the number of layers, we observe a red shift in the frequency of the mode, whereas its damping rate remains unchanged. The experimental frequency shifts with sample thickness can be explained surprisingly accurately using zone folding of the graphite phonon dispersion relation. [1] T. Mishina et al., Phys. Rev. B 62, 2908 (2000) [2] S. K. Saha et al., Phys Rev. B 78, 165421 (2008)

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### Edge effects on vibrational dynamics of graphene nanoribbons and nanoflakes

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The amazing thermal properties of GNRs have oriented many works on their phonon features. Using Raman spectroscopy, GNR vibrational dynamics were shown to be strongly dependent on the proximity and shape of edges (armchair or zigzag) [1]. These properties have been recently investigated theoretically using first-principle approach [2] but lots of questions are still opened. In this work, the force constant model including fifth-nearest neighbor atoms [3] was used to calculate the phonon dispersion and the vibrational density of states (VDOS) of semi-infinite GNRs and nanoflakes of various width and edge orientations. Besides typical graphene peaks like E2g (G peak) and D, we clearly identify several distinctive ribbon peaks in ribbon VDOS depending on the edge shape. In particular, most of armchair modes have been detected at about 1350cm-1 and 1480cm-1, associated with strong localized in-plane vibrations, and at about 630cm-1, associated with out-of plane vibrations. Typical armchair and zigzag peaks have been also observed when introducing edge disorder. The VDOS corresponding to the above mentioned specific modes gradually decrease if the number of discontinuities per periodic unit cell increases with respect to the perfect structure. Therefore, the edge nature can be identified by detecting the characteristic ribbon peaks in the VDOS and the peak intensity provides information about the quality of the edge shape. [1] L.G Cançado et al., Physical Review Letters 93 247401, 2004. [2] R. Gillen et al., Physical Review B 80 155418, 2009. [3] M. Mohr et al., Physical Review B 76 035439, 2007.

## Poster Board | 61

### Mechanism of carbon nanotubes unzipping using lithium and ammonia intercalation

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Graphene nanoribbons (GNRs) are important due to their fascinating physico-chemical properties. Recently, viable, large scale and low cost routes, involving the unzipping of carbon nanotubes have been reported. These unwrapped tubes could exhibit a large number of applications based on their edge morphology, width, and surface chemical modification. These applications include the fabrication of nanoelectronic devices, nanosensors, photonic and nanomechanical devices. Different routes to unzip these tubes have been reported, but their formation mechanisms are still far from clear. In this report, using a density functional theory (DFT) and force field calculations (FFC) under different temperature parameters, we computed the interaction between a double-wall nanotube (DWNT) intercalated with lithium ions and ammonia molecules. We have observed an inter-walled expansion in a DWNT which is similar to the one reported experimentally between graphene sheets, apparently, intercalated with NH3 or Li. These graphite and nanotube intercalated models, have then been used to simulate exfoliation experiments reported by Cano-Márquez et al., that resulted in the formation of exfoliated multi-walled carbon nanotubes (Ex-MWNT), or GNRs. We also studied the possibility to accumulate sufficient mechanical stress within the walls of the nanotubes in order to unzip the nanotubes and form ribbons.

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### Electron and optical phonon temperatures in electrically biased graphene

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Graphene layers, owing in part to their ability to sustain very high current densities, are foreseen for novel applications in nanoscale electronic and optoelectronic devices. Under high electrical bias the current in a graphene channel has been shown to exhibit saturation behavior [1,2], which is intimately related to the energy dissipation mechanisms in graphene. Here we present an in situ study of the intrinsic energy dissipation steps in graphene field effect transistors operating in the high-current regime. By combining an original approach based on the analysis of the thermal radiation from graphene and a Raman spectroscopy study, we obtain, respectively, independent determinations of the electron and the optical phonon temperatures [3]. We find that these two populations are in thermal equilibrium, with temperatures in excess of 1500 K for dissipated electrical powers of ~500 kW/cm2. For a given optical phonon temperature, the anharmonic downshift of the Raman G-mode is smaller than the value expected under equilibrium conditions, suggesting that these high-energy optical phonons may not be in full equilibrium with the graphene lattice. References: [1] I. Meric et al., Nat. Nanotechnol. 3, 654 (2008). [2] A. Barreiro et al., Phys. Rev. Lett. 103, 076601 (2009). [3] S. Berciaud et al. (submitted)

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### Quantitative & Qualitative Analysis of Various Surfactant-Exfoliated Graphene Dispersions

**Ronan Smith**, *School Of Physics, Trinity College Dublin, Ireland; CRANN, Trinity College Dublin* | **Mustafa Lotya**, *School Of Physics, Trinity College Dublin, Ireland; CRANN, Trinity College Dublin* | **Paul King**, *School Of Physics, Trinity College Dublin, Ireland; CRANN, Trinity College Dublin* | **Jonathan Coleman**, *School Of Physics, Trinity College Dublin, Ireland; CRANN, Trinity College Dublin*

Recent work has shown a method to disperse and exfoliate graphite to give graphene suspended in water-surfactant solutions[1,2] This process has many advantages over solvent based exfoliation[3] including bio-compatibility, safe processing and low cost. Very few surfactants have been tested for this process and very little work has been done to compare different types of surfactant with a view to optimization of dispersion yield and quality. In this work, graphite has been exfoliated to give graphene using various anionic, cationic and non-ionic surfactants. 12 surfactants are compared based on their exfoliation efficiency at a fixed low surfactant concentration. The dispersion yields are compared using absorption spectroscopy while dispersion quality is assessed using TEM and Raman Spectroscopy. References [1] Lotya et al. Journal of the American Chemical Society 2009, 131, 3611. [2] Green et al. Nano letters 2009, 9 (12), 4031. [3] Hernandez et al. Nature Nanotechnology 2008, 3, 563.

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### Percolation in size distributed carbon nanotubes mats

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Carbon nanotubes mats (CNTMat) with various degrees of structural organization have promising electric properties that compare with those of actual transparent electrodes used in electroluminescent and photovoltaic devices. The optimization of such complex materials and the description of the underlying physics can be efficiently addressed by computational means. For example, the modeling of charge transport in such complex systems improves our understanding of the influence of the network structure on the quality of the electrode, and contributes to selectively optimized the electrode properties. The charge transport models already developed for CNTMat typically consider a single parameter to describe the tube-tube junctions [1]. However, it has been recently shown that the propagation of charge carriers is limited by contact resistance which is far from being unique in CNTMat where nanotubes have various physical properties [2]. We have developed Monte Carlo algorithms simulating the charge transport in bidimensional networks of carbon nanotubes that incorporate a realistic distribution and description of tube-tube junctions. The algorithms generate random networks, check for percolation paths and evaluate the total conductance of the CNTMat on the basis of individual contacts conductances, which in turn depend on the local network properties. We will present different results in which the importance of the nanotube distribution on the resulting electrical performances can be described in terms of length, diameter, orientation and chirality of the nanotube distribution within the percolative network. [1] J. Hicks et al., Phy. Rev. E, 79, (2009). [2] P. N. Nirmalraj et al. Nano Lett., 9, (2009).

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### Critical current 0-Pi transition in a single wall carbon nanotube SQUID

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Nanotube quantum dots (QD) allowed exciting achievements such as Wigner crystals, SU(4) Kondo effect and many more including superconducting junctions. A single wall carbon nanotube (SWNT) in a resonant tunneling conduction regime between two superconductors realizes a Josephson quantum dot junction. In a transistor-like configuration, it is possible to tune the critical current of the Josephson junction with the gate [1]. Such a junction exhibits two manifestations of electronic correlations: Kondo effect for an odd number of electrons on the QD and superconductivity. The interplay between these two competing phenomena can give rise to peculiar properties such as a Pi dephasing of the Josephson current-phase relation (Pi-junction) [2]. In this work, we focus on the 0-Pi transition of SWNT Josephson QD junctions. Theory predicts the Josephson QD junction behaviour is determined by the ratio delta/TK, where the temperature TK scales the Kondo effect, while the energy gap delta scales superconductivity [3]. For this purpose, we have built a Superconducting Quantum Interference Device (SQUID), the weak links of which are realized by two portions of a SWNT [2]. Such geometry allows tuning delta/TK and measuring directly the Pi-dephasing in the magnetic field modulation of the switching current. We have monitored the 0-Pi transition depending on delta/TK. Our experiments confirm theoretical predictions and provide a new control over the SWNT-Josephson QD junctions. [1] P. Jarillo-Herrero et al., Nature 439, 953 (2006). [2] J.-P. Cleuziou et al., Nat. Nanotech. 1, 53 (2006). [3] C. Karrasch et al., Phys. Rev. B 77, 024517 (2008).

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### Devices from sorted carbon nanotubes: From hydrogen sensing to electroluminescence

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We have recently combined techniques for sorting and assembling of carbon nanotubes to fabricate device arrays from sorted single-walled carbon nanotubes[1]. Here we report on the hydrogen sensitivity of Schottky-barrier field effect transistors from (n,m)-sorted semiconducting single-walled carbon nanotubes in contact with Pd electrodes. We observe an unexpected dependence of the hydrogen sensitivity on the nanotube diameter, with maximum sensitivity for devices from (9,7) nanotubes and no sensitivity for devices from (6,5) nanotubes[2]. For (9,7)-devices the conductance changes by two orders of magnitude at 100ppm H2. We will also report on electroluminescence from metallic SWNTs, MWNT and FLG devices[3]. SWNT devices were assembled from tubes with different diameters ranging from 0.7-1.5 nm. We observe diameter-independent light emission in the visible spectrum with peaks at 1.4 and 1.8 eV. Similar peaks are observed for MWNT and FLG devices. We propose that the light emission is due to phonon assisted radiative decay from populated p* band states at the M point to the Fermi level at the K point. [1] "Towards Single-chirality Carbon Nanotube Device Arrays", Vijayaraghavan, Hennrich, Stürzl, Engel, Ganzhorn, Oron-Carl, Marquardt, Dehm, Lebedkin, Kappes, Krupke, submitted 2010. [2] "Hydrogen sensing with chirality sorted carbon nanotubes", Ganzhorn, Vijayaraghavan, Dehm, Hennrich, Fichtner, Voigt, v. Löhneysen, Kappes, Krupke, 2010, patent pending. [3] "Phonon assisted electroluminescence from metallic carbon nanotubes and graphene", Essig, Marquardt, Vijayaraghavan, Ganzhorn, Dehm, Hennrich, Ou, Green, Sciascia, Bonaccorso, Bohnen, v. Löhneysen, Kappes, Ajayan, Hersam, Ferrari, Krupke, submitted 2010.

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### Integration of Carbon Nanotube Devices in an Optical Microresonator

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In recent years electron-phonon coupling (EPC) in single-walled carbon nanotubes (SWCNT) has spurred great interest both experimentally and theoretically. Appreciable EPC ultimately limits the high field transport in metallic SWNT when electrons above a certain energy threshold (~0.2eV) scatter with optical phonons[1]. Therefore, it is desirable to control the phonon population in SWNT devices. Recent experiments have shown that it is possible to enhance/inhibit specific phonons of isolated SWNT immobilized inside a planar optical Lambda/2-microresonator[2]. Here we demonstrate a reliable process to integrate SWNT devices in an optical microresonator cavity. Our approach combines standard nanofabrication techniques with low frequency dielectrophoresis (DEP) and atomic layer deposition. First, contacts are defined on a freestanding 50nm Si3N4 membrane onto which metallic SWNT are deposited by DEP from a metallic SWNT enriched solution. Then a thin dielectric layer of Al2O3 is deposited. Finally, silver is evaporated on both sides of the samples that act as mirrors. The thickness of the dielectric layer is chosen according to our simulations based on a standard transfer matrix approach to match a desired resonance wavelength. The resonance wavelength of the microresonator cavities is characterized by FTIR. Initial Raman scattering experiments on half-cavity samples already show improved sensitivity for Anti-Stokes Scattering of phonons limiting high field transport. [1] Yao, et al., Phys. Rev. Lett., 2000, 84, 2941 [2] Steiner, et al., Nano Lett., 2007, 7(8), 2239

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### Electron transport of meso-scale carbon nanotube-based materials at the finite temperature

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We have investigated electron transport of carbon nanotube at the finite temperature through the large scale simulation using high-end supercomputer. For our research, we have developed an advanced tight-binding molecular dynamical method based on a non-equilibrium Green's function at the finite temperature for simulating the electrical conduction through electrodes. Avoiding heavy loads in computing, our O(N) approach of algorithm enables us to simulate the meso-scale electrical quantum transport phenomena with several ten thousands of carbon atoms. It results that the current flux at each atomic point of a single-walled nanotube strongly depends on the condition of electrodes to which the carbon nanotube is connected at both ends. As the quantum effect on current flux, it shows that the relation of current-voltage is distinct from that of the classical transport defined by Ohm's law. The difference gradually disappears with increasing temperature because the quantum effect is weakened. In addition to a single walled nanotube, we will discus the electron transport properties of a double wall and twisted bundle carbon nanotubes.

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### Nature of the metallic ground state in intercalated metallicity selected single wall carbon nanotubes

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In this contribution we present recent results on the details of the electronic properties of intercalated metallicity selected single wall carbon nanotubes buckypaper samples using high energy spectroscopy as probe. Interestingly, for bundles of metallic tubes the ground state of a 1D metal is still preserved. The consequences of doping on the nature of the metallic ground state in bundles of metallic tubes as well as the semiconductor to metal transition in semiconducting tubes are elucidated in detail. Special emphasis will be given on the intercalation dependent change of the interaction between the metallic tubes in a bundle, yielding a transition of the 1D metallic Tomonaga-Luttinger liquid ground state to a normal 3D Fermi liquid. The impact of these results in accessing the maximum conductivity in carbon based conducting transparent electrodes will be discussed. Work supported by the DFG projects PI 440 3/4/5 and FWF project P21333-N20.

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### Structural analysis of titanium dioxide nanotubes

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Based on experimental evidence we propose in this work an alternative structure to those reported in the literature about the formation of titanium dioxide nanotubes (TiO2NTs). We builded nanotubes with inner diameter ranging from 13 to 50 Å and from layers of atoms extracted from the crystalline structure of titanium dioxide in anatase form. Layers were used containing 1, 2 and 3 crystal planes (101). Two experimental evidences give support to this proposal. Experiments have shown that the cleavage of the crystal of titanium dioxide in anatase form is facilitated in the direction of the plan (101).[1] Further results of X-ray diffraction in TiO2Nts samples point to a greater occurrence of the plane (101) in this structure.[2] Molecular mechanics calculations indicate that the energy of formation is inversely proportional to the diameter of the tube, as already obtained in other proposed structure. [3] The best results were obtained for symmetrical tubes with axis along [010] direction. Semi-empirical calculations performed in arcs from such tubes remained fixed ends confirmed the inverse proportionality between energy and diameter. References [1] IWAKI, T. J. Chem. Soc., Faraday Trans. 1, v. 79, p. 137–146, 1983. [2] KASUGA, T. et al. Langmuir, v. 14, p. 3160–3163, 1998. [3] WANG, J. et al. Physica E, v. 41, p. 838–842, 2009. "

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### Electronic transport through a folded graphene nanoribbon

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Studies of annealed graphite using high resolution TEM images show a predominance of closed edges between layers of graphene and a large proportion of AA stacking [1]. In this work we present a theoretical study of transport properties of a system formed by a folded edge bilayer graphene nanoribbon with nanoribbon contacts. Geometric and electronic properties of similar systems composed by two flat graphene layers continuously connected by a fractional nanotube have been studied before by J. Feng et al. [2]. We consider two configurations obtained by folding a monolayer ribbon in two different forms: in one the monolayer nanoribbon is folded in such a way both ribbon segments are set one on top the other, in the second configuration the ribbon segments of the bilayer are oriented in an angle of 60° with respect to the other. In both cases the graphene segments of the nanostructure are in AA stacking order. We show calculations of the local density of states, linear conductance as a function of structural. The system is described by a pi-band TB Hamiltonian with nearest-neighbor interaction. The interlayer coupling is modeled with single hopping connecting atoms directly on top of each other. The electronic and transport properties are calculated using the Green's function method with real space renormalization techniques and the Landauer formalism. [1] Z. Liu, et al, Phys. Rev. Lett. 102, 015501 (2009). [2] Ji Feng, et al, Phys. Rev. B 80, 165407 (2009).

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### Electrical and Optical Properties of Covalently Functionalized Double-Walled Carbon Nanotubes

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Double-walled carbon nanotubes (DWNT) present a particular geometry in which the inner wall is isolated by the outer wall, while the latter is in direct interaction with the environment. Here, we studied optical and electrical properties of functionalized DWNT derivatives (f-DWNT) prepared by aryldiazonium reactions. We first present absorption spectra of f-DWNT films and resonant Raman spectra of individual f-DWNT assembled in devices. The results show that the functionalization reaction occurs only at the surface of the outer wall, leaving the properties of the inner wall intact. Second, electrical transport experiments performed on individual f-DWNT field-effect transistors revealed that the inner wall carry electrical current with a similar intensity as for a single-walled carbon nanotube. Finally, we demonstrate that simple electrical measurements combined with covalent functionalization are sufficient to determine the metallic or semiconductor character of both walls.

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### Electronic and Magnetic Properties of Carbon/Boron-Nitride Heterojunction Zigzag Nanoribbons

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First-principles calculations using density functional theory are carried out in order to investigate the electronic and magnetic properties of zigzag nanoribbons formed by different segments of carbon and boron-nitride (heterojunction nanoribbons). All nanoribbons were relaxed using conjugate gradient algorithm. For all systems, the electronic density of states, the binding energy, and the magnetic states were analyzed as a function of the width of the nanoribbon and the segment length of the carbon and boron-nitride. Different spin density distributions were considered as starting configurations in order to determine the magnetic ground state. We found that the most stable spin configuration depends strongly on the C and BN segment lengths. For specific widths, interesting results on structural transformations were obtained; pentagonal and heptagonal rings appear at the edges losing the magnetic behavior. It has been found that in the absence of these defects, the hexagonal lattice dominates the structure in zigzag nanoribbons exhibiting a magnetic state, which consists of spins localized at the atom edges. Here, the edge dominated by carbon and boron present antiparallel spins (antiferromagnetism) whereas the edge dominated by carbon and nitrogen exhibits parallel spins (ferromagnetism). In addition, for some cases, half-metallic behavior has been found. The adsorption of gases in these nanoribbons is analyzed in order to be used as toxic gas sensor.

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### Vacancies and Nitrogen-Doped Effects on the Electronic and Structural Properties of the (10,0) Semiconducting Carbon Nanotube

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The electronic and structure reconstruction properties as a function of the number of vacancies and nitrogen concentration on the (10,0) single walled carbon nanotubes are investigated using first-principles density functional theory and the local density approximation. In particular, we introduce one and two vacancies and the low coordination atoms (pirydine-like sites) were substituted by nitrogen atoms. We explore all possible ways of setting one or more nitrogen atoms at the pyridine-like sites. All structures were relaxed using conjugated gradient method. We calculated the electronic density of states, the electronic band-gap, and the binding energy. We found that carbon nanotubes can be changed from semiconductor to metallic modifying the concentration and position of nitrogen surrounding the vacancy. It has observed after structure relaxation a self-reconstruction in the surface if two adjacent vacancies are introduced in the tube, creating a corrugated surface with local formation of pentagonal and octagonal rings.

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### High performance polymer nanofiltration membranes produced by optimizing dispersions of Carbon Nanotubes in different solvents

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Despite the outstanding mechanical and electrical properties of individual carbon nanotubes, industrial applications for MWCNT are just in the early stage of development. One big open issue – not only but especially for the research on CNT-polymer composites – is the dispersion of nanotubes in solvents or polymer matrices. Breaking the CNT agglomerates, removing catalyst particles and amorphous carbon and finally bringing the individualised MWCNT into a stable dispersion are the crucial steps in producing CNT-polymer composites. In this work, dispersions of MWCNT in aqueous solutions and organic solvents were produces by using different techniques. The most common technique of ultrasonic treatment was compared with high pressure dispersion, ball mill and rotor/stator-dispersion. The influence of different parameters like temperature, power, or viscosity of the solvent was studied. For the latter, aqueous solutions of polyvinylalcohol (PVA) with different molecular weight were produced. The dynamic viscosity was measured by rheometry and was brought in context with the dispersability of CNT. The degree of dispersion was evaluated by measuring PVA-CNT composites by thermo gravimetric analysis (TGA). Using the results of these measurements, CNT-polysulfone composite nanofiltration membranes were fabricated. Characterization using TGA, SEM, and porometry held pore sizes between 20nm and 80nm and electrical conductivity up to almost 1 S/m. Permeability, separation behaviour and a possible heating effect on membrane and fluid were studied. The results show the importance of dispersion quality on properties of CNT polymer composite. The approaches of increasing dispersability are serviceable for many fields of CNT research and application.

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### Enhancing the mechanical performance of carbon nanotube fibres

**Slawomir Boncel**, *University of Cambridge, United Kingdom; Silesian University of Technology, Poland* | **Rajyashree Sundaram**, *University of Cambridge, United Kingdom* | **Ahu Dumanli**, *University of Cambridge, United Kingdom* | **Alan Windle**, *University of Cambridge, United Kingdom* | **Krzysztof Koziol**, *University of Cambridge, United Kingdom*

Despite the potential applications in niche areas, carbon nanotubes (CNTs) have to yet make the transition from science to realistic technology. The excellent mechanical properties of individual carbon nanotubes are not very easily scalable in macroscopic assemblies, like carbon nanotube based fibres and films. Very high mechanical properties have been observed in carbon nanotube fibres at few millimetres gauge length (1). The two key strategies for enhancement of strength are increases in the length of the individual nanotubes and increasing the stress transfer between them through shear forces. Further enhancement in nanotube length is difficult to achieve and thus we have focused on enhancement of the shear interaction between neighbouring bundles of nanotubes. Chemical cross-linking of the CNTs within a fibre has a tremendous potential and could be the solution for the requirements of very long nanotubes. The process was successfully developed by application of various bifunctional organic molecules towards reactive sides of CNTs and numerous organic side products of a CVD process. A scouting cross-linking experiment carried out on as made CNT fibres demonstrated two-fold increase in the specific strength, increase in stiffness and remarkable increase in toughness of the fibre after the treatment. Furthermore, the uniformity of the fibre performance is worth noticing. (1) K. Koziol, J. Vilatela, A. Moisala, M. Motta, P. Cunniff, M. Sennett, A. Windle, 'High performance carbon nanotube fiber', Science, 318 (2007), 1892-1895.

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### Aligned Carbon Nanotubes Carpets by aerosol assisted CCVD for nanomembranes

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Carbon Nanotubes exhibit remarkable molecular and ionic transport properties [1]. These properties gave birth to great hopes for preparing high flux and high selectivity membranes for nanofiltration made of dense and aligned carbon nanotubes carpets [2][3]. Numerous simulation predicted a dramatic enhancement of waterflow inside small diameter nanotubes and first experiments have demonstrated an enhancement factor regarding classical transport laws more than three decade higher [4]. Francis Perrin Laboratory developped an aerosol assisted Catalytic Chemical Vapour Deposition method to grow Carbon Nanotubes Carpets in a single step process. This technique open the way to a robust and large area process that could produce large scale carpet [5]. But it is important to be sure that this process allow to produce nanotubes that meet the specifications for making good membranes. The second step consist to fill the inter tube spaces with a non permeable matrix which do not modify the quality of the carpet. The last step aims at opening the tubes. We present our latest results regarding the ability to prepare Aligned Carbon Nanotubes based Membranes of different features, the caracteristation of each step of the process and draw the main obstacles that should be overcome to pave the way to real application. References [1] Smith, B. W et al. Nature, 1998 [2] Hummer et al. Nature 414, (2001) [3] B. Corry et al.; J. Phys. Chem. B, 112, 2008 [4] Hinds, B. et al., Science 303, (2004) [5] M. Pinault et al., Nano Letters 5 (2005)

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### Studying the Mechanical Properties of Carbon Nanotube Fibers for Energy Storage Applications

**Frances Hill**, *Massachusetts Institute Of Technology, USA* | **Timothy Havel**, *Massachusetts Institute Of Technology, USA* | **A. John Hart**, *University of Michigan* | **Carol Livermore**, *Massachusetts Institute Of Technology, USA*

With exceptional mechanical properties, including a high Young's modulus of 1 TPa and the ability to sustain large elastic strains, carbon nanotubes (CNTs) offer considerable potential as a material for energy storage [1]. Mechanical springs made of densely packed bundles of CNTs loaded to 15% tensile strains are expected to store energy with a density of 7.7 × 106 kJ/m3 or 5000 kJ/kg, higher than the volumetric and gravimetric energy density of lithium ion batteries and three orders of magnitude higher than the energy density of steel springs [2]. Fibers are fabricated as representative springs from multi-wall CNTs grown by thermal chemical vapor deposition and their mechanical properties and energy storage capabilities are tested. Each fiber is prepared by pulling a small strand of CNTs from the side of a forest. The initial low density of the fibers of 0.02 g/cm3 is increased to maximize volumetric energy density and improve the structural cohesion of the CNTs within the fibers. The present work compares the effects of densification using twisting, capillary-driven densification, and a combination of both techniques on the performance of the springs under tensile loading. The results show that twisting lowers both the strength and stiffness of the fibers, while capillary-driven densification increases both the strength and stiffness of the fibers. A displacement stage built inside of a scanning electron microscope provides additional valuable insights into the behavior of CNT fibers during tensile loading and failure. [1] Hill et al., Micromech. Microeng. 19 [2] Hill et al. Nanotechnology 20

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### Dependence of electrical resistance of carbon nanotube proto yarn on force

**Agnieszka Lekawa-Raus**, *University of Cambridge, United Kingdom* | **Krzysztof Koziol**, *University of Cambridge, United Kingdom* | **Alan Windle**, *University of Cambridge, United Kingdom*

A significant practical problem in assessing the performance of many fibres and yarns arises from the difficulty of knowing their exact diameter. This has been overcome in the fibre industry through the use of the unit of tex which is the mass in grams of a kilometre of fibre, so the strength as specific stress (GPa/SG) is measured in terms of the breaking load per unit tex (N/tex). For yarn-like electrically conducting fibres the same problem exists so we use a specific conductivity, Sigma= G x l / LD which is conductance (G) multiplied by length (l) and divided by linear density (LD) given in unit tex=g/km, and thus can be measured much more reliably than classical conductivity. The electrical properties of carbon nanotube proto yarns have been measured as a function of applied strain. Specific conductivity depends on both elastic and plastic strain, although much more strongly on the former. In each case, although reversibly for elastic dependent on, the change in specific conductivity can be attributed to a change in internal structure of the proto yarn on extension. An outline model is proposed.

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### Carbon nanotube reinforced carbon composites

**Nagore Ibarra-Gonzalez**, *University of Cambridge, United Kingdom* | **Alan H. Windle**, *University of Cambridge, United Kingdom*

Carbon-carbon composites are interesting materials due to their combination of low weight with potentially excellent physical properties such as strength, stiffness, thermal conductivity and/or electrical conductivity. In addition, the magnitude of these physical properties remains relatively high even at extreme temperatures (>1100°C). The thermal conductivity of commercially available carbon fibre- carbon composites is in the order of 350 W/mK at room temperature. In this context, carbon nanotubes, which show thermal conductivity values of 1000 W/mK and above, have been previously proved to contribute positively when incorporated within carbon-carbon composites. In the present work, thermal and mechanical properties of novel anisotropic carbon nanotube-carbon composites will be presented and their viability as materials for heat removal applications (ranging from nuclear components to heat sinks in electronic devices) will be discussed.

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### Lifetime Evaluation of Carbon Nanotube Field Emitters by ink-jet printing

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Carbon nanotube(CNT) as a field emitter has been extensively investigated to apply for light sources. CNT emitters were fabricated by an ink-jet printing using the ink with thin multiwall carbon nanotube(MWCNT). First, we deposited the indium as an adhesive metal layer by thermal evaporator on ITO coated glass substrate. And then, the MWCNT ink was directly dot-patterned onto the substrate by the ink-jet printing. The patterned substrate was thermally annealed for the physical bonding between MWCNTs and indium layer, followed by the treatment with O3 to obtain the uniform length of CNT emitters. Afterwards, it was packaged under vacuum ambient with a frit glass with an anode which is an ITO coated glass without any phosphors to evaluate the absolute lifetime of CNT emitters. We investigated the field emission properties and the lifetime of CNT field emitters under about 10-6 torr. We could know that the lifetime of CNT field emitters obtained by ink jet printing were much more than 100 hours at current density of 600.

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### Piezoresistive acoustic sensors based on inkjet printed carbon nanotube network

**Kyoung Il Lee**, *Korea Electronics Technology Institute, Korea; Seoul National University* | **Sang Un Byun**, *Korea Electronics Technology Institute, Korea* | **Jong Hun Han**, *Korea Electronics Technology Institute, Korea* | **Kwon Woo Shin**, *Korea Electronics Technology Institute, Korea* | **Seong Hyun Kim**, *Korea Electronics Technology Institute, Korea* | **Chul Seung Lee**, *Korea Electronics Technology Institute, Korea* | **Yongtaek Hong**, *Seoul National University*

Carbon nanotube pattern was inkjet-printed on a boundary of BCB(Benzocyclobutene) diaphragm with a water-based ink containing multi-walled carbon nanotube. A commercial inkjet printing system includes a glass capillary type piezoelectric inkjet head with a nozzle of 50 um inner diameter. The BCB diaphragm was made on a silicon wafer by deep silicon etching process. The diameter of the diaphragm is 2 mm and the overall size of the chip is 3 mm x 3 mm x 0.5 mm. The carbon nanotube patterns are connected to bonding pads by silver electrodes printed by inkjet printing. The size of the carbon nanotube pattern is about 100 x 300 microns and the resistance of the pattern varies from 50 kOhm to 500 kOhm, depending on the number of printing. Since the carbon nanotube has a piezoresistivity, the resistance of the carbon nanotube pattern changes as the applied sound pressure deforms the diaphragm and carbon nanotube on it. It shows about 20 uV output voltage with a 18 V bias voltage for a sound pressure of 1 Pa at 20 kHz. The sensitivity is very low even at the resonance, so the device cannot be used as a omni-directional microphone with a flat frequency response over the entire audible range. But its small size comparing to the conventional ultrasonic sensors and the simple fabrication process comparing to the capacitive MEMS microphone requiring more than 7 photo-lithography steps, can be very attractive and we expected the application of direction sensors.

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### Cantilevered carbon nanotubes as mechanical oscillators

**Takayuki Arie**, *Osaka Prefecture University, Japan; CREST-JST* | **Shun Fukami**, *Osaka Prefecture University, Japan* | **Seiji Akita**, *Osaka Prefecture University, Japan; CREST-JST*

Carbon nanotube cantilevers are suitable for mass and force sensors using their outstanding resonant characteristics. However, the details on their resonance remain to be elucidated. In this study, we present the gaseous pressure and temperature dependences of nanotube oscillations using our optical detection technique and scanning electron microscopy. The quality factor of the nanotube oscillation was inversely proportional to the pressure at 100-10000 Pa, in which the fluid is in the free molecular regime. In contrast, at pressures below 10 Pa the quality factor was constant, suggesting that the energy loss induced by the gas molecules is much less than the intrinsic oscillation energy loss. This is because the mean free path of air is much greater than the nanotube diameter. To explore the temperature dependence of the oscillation, we measured the resonant frequencies of the nanotubes synthesized by arc-discharge and chemical vapor deposition at various temperatures. The nanotube by arc-discharge showed the maximum resonant frequency at 150 K, while the nanotube by chemical vapor deposition showed at 100 K. Furthermore, the quality factor showed the same trend for each type of nanotubes. The difference in temperatures showing maximum values is possibly attributed to the crystallinity of the nanotubes synthesized by different processes, consistent with our results from molecular dynamics simulation.

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### Wave Front Velocity Oscillations of Carbon Nanotube-Guided Thermopower Waves: Nanoscale Alternating Current Sources

**Michael Strano**, *Massachusetts Institute Of Technology, USA* | **Joel Abrahamson**, *Massachusetts Institute Of Technology, USA* | **Wonjoon Choi**, *Massachusetts Institute Of Technology, USA* | **Jae-Hee Han**, *Massachusetts Institute Of Technology, USA* | **Kourosh Kalantar-Zadeh**, *Royal Melbourne Institute of Technology University*

The nonlinear coupling between exothermic chemical reactions and a nanowire or nanotube with large axial heat conduction results in a self-propagating thermal wave guided along the nano-conduit. The resulting reaction wave induces a concomitant thermopower wave of high power density (> 7 W/g) resulting in an electrical current along the same direction. We develop the theory of such waves and analyze them experimentally, showing that for certain values of the chemical reaction kinetics and thermal parameters, oscillating wave front velocities are possible. We demonstrate such oscillations experimentally using a cyclotrimethylene-trinitramine/multiwalled carbon nanotube system, which produces frequencies in the range of 400 to 5000 Hz. The propagation velocity oscillations and the frequency dispersion are well described by our theoretical calculations and are linked to oscillations in the voltage generated by the reaction. These thermopower oscillations may enable new types of nanoscale power and signal processing sources.

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### Carbon nanotube: A low-loss spin-current waveguide

**Mauro Ferreira**, *Trinity College Dublin, Ireland* | **Filipe Guimaraes**, *Universidade Federal Fluminense, Brazil* | **Antonio Costa**, *Universidade Federal Fluminense, Brazil* | **Roberto Muniz**, *Universidade Federal Fluminense, Brazil* | **Doug Mills**, *University of California at Irvine, USA*

We demonstrate with a quantum-mechanical approach that carbon nanotubes are excellent spin-current waveguides and are able to carry information stored in a precessing magnetic moment for long distances with very little dispersion and with tunable degrees of attenuation. Pulsed magnetic excitations are predicted to travel with the nanotube Fermi velocity and are able to induce similar excitations in remote locations. Such an efficient way of transporting magnetic information suggests that nanotubes are promising candidates for memory devices with fast magnetization switchings.

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### Interaction of a Single-Walled Carbon Nanotube with PMMA

**Meysam Rahmat**, *McGill University, Canada* | **Pascal Hubert**, *McGill University, Canada*

Mechanical performance of a nanocomposite is influenced by the properties of the reinforcement and the matrix, and also by the interaction between them. The interaction properties play a significant role in load transfer and dispersion in nanocomposites. Therefore, the objective of this work is to investigate the carbon nanotube – polymer interaction in nanocomposites. The interaction between Polymethylmethacrylate (PMMA) and a Single-Walled Carbon Nanotube (SWNT) was studied by modelling and experiments. The modelling approach was performed using Molecular Dynamics (MD). The MD software LAMMPS was used to run the simulations. First, independent MD models of carbon nanotubes and PMMA chains were created. The MD models were validated by simulating physical properties, and the results were in accordance with literature. Secondly, the SWNT and PMMA models were combined and a three-phase simulation was carried out to study the SWNT – PMMA interaction. The interaction energy was calculated and found to agree with the literature. The experimental investigations of the interaction properties were performed by Atomic Force Microscopy (AFM). The chemical force microscopy technique was employed. The AFM probes were functionalized with PMMA, and a sheet of SWNT buckypaper was used as the substrate. In order to evaluate the functionalization procedure, the AFM probes were inspected with a Scanning Electron Microscope before and after the process. The interaction properties of the system were studied through AFM force curves obtained under water. The experiments, along with the MD simulations, create a framework to understand the interaction at the nanoscale.

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### H2/H+ interconversion reactions through the chemical derivatization of carbon nanotubes with a bio-inspired hydrogenase mimic

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Among the new energy technologies, the use of hydrogen is an attractive solution. However, the hydrogen energetic chain must produce hydrogen in large quantities by hydrolysis of water in devices called electrolyzers, and secondly use hydrogen in fuel cells to provide energy by its oxidation. Currently these processes require using platinum as a catalyst. However, this metal is extremely rare and therefore very expensive. Getting rid of platinum and developing efficient materials that contains only abundant and cheap elements is a major challenge for the future of the hydrogen energetic chain. To substitute platinum by abundant and low cost metals, researchers look at the chemical processes at work in living organisms which know how to use hydrogen as an energy source, or to produce it from water from abundant metals like iron and nickel. That bio-inspired approach which tries to reproduce those natural processes involves the synthesis of compounds based on nickel and iron mimicing the hydrogenase enzymes present in biosystems. We present the catalytic activity for both the production and the uptake of hydrogen of nickel-based bio-inspired catalysts covalently bent on carbon nanotubes. This extremely stable material operates in highly acidic environment and is compatible with the Nafion® membranes. The development of this new material represents a new stage in the race for the improvement of the hydrogen solution for energy. 1- A. Le Goff, V. Artero, B. Jousselme, P. D. Tran, N. Guillet, R. Metaye, A. Fihri, S. Palacin, M. Fontecave, Science, 2009, 326, 1384.

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### Development of optical responsive carbon nanotubes cell cultured substrate

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Single-walled carbon nanotubes (SWNTs) are nanomaterials that possess remarkable electrical, mechanical, and thermal properties and have been explored for biological applications. One of the applications of SWNTs in biology is the cell culture substrate, where the unique one-dimensional high aspect structure and hydrophobic nature of SWNTs gave better substrate to culture the cells. In this report, we describe the novel concept of photo active SWNTs dish for selective cell collection. SWNT-coated cell culture substrate was fabricated using the spray coating method. Slightly grayish color on glass substrate indicates the thin coating of the SWNTs and SWNTs network structure was clearly seen in AFM image. Compared to the HeLa cells cultured on the non-coated dish, SWNT-coated dish lead the similar cellular proliferation rate as well as the adhesion morphology for HeLa cell culturing. We observed selective removal of HeLa cells by the near-infrared (NIR) irradiation of the substrate. We assumed that the mechanism of the cell removal is the photoacoustic effect of SWNTs and the collapse of SWNTs substrate. By reducing the water layer above the cell, irradiated cells were successfully flied out from the medium and captured at the top lid of the dish. Cell viability after NIR irradiation was estimated by the MTT assey. It suggested that the HeLa cells removed after NIR irraidiation are still viable and this selective removal method have no influence on the proliferation rate of the cells.

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### Growth and fabrication of carbon nanotubes and graphene devices towards gas sensor applications

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Graphene and carbon nanotubes are amongst the most interesting and studied materials nowadays. Both of them are composed of sp2 carbon bonds that inherit several important properties of graphite, namely high in-plane electrical conductivity, thermal conductivity and mechanical strength. In this work, I will present the recent advances towards the growth and fabrication of carbon nanotubes and graphene devices for sensor applications. SWCNTs were grown on silicon substrates by thermal chemical vapour deposition (CVD). Iron (Fe) was chosen as the catalyst metal to promote CNT growth. Two different configurations were used to obtain a high yield of SWCNT. Firstly, Fe thin film (~ 1 nm) is deposited directly on the SiO2/Si substrate. Secondly, the same Fe film is deposited on Al(10nm)/SiO2/Si substrate. Graphene and few-layer graphene samples were prepared using different methods: 1) Standard exfoliated procedure was performed using semiconductor grade tape and then characterized using a combination of optical microscopy, atomic force microscopy (AFM) and Raman spectroscopy. To remove tape residue the graphene samples are heated in a quartz tube at 500°C for 15min under Ar:H2 flow (850:150 sccm). 2) Epitaxial graphene were grown using a home made directed current furnace (500 sccm Ar – 1800 oC) using different orientations of SiC substrates. Back gated field effect transistor devices based on isolated carbon nanotubes and graphene were prepared standard photo-lithography and evaporation techniques. Results showing the response of the devices exposed to different gases such as hydrogen, oxygen, humidity and water will be presented.

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### Diffusional motion analysis of water-dispersible and uniform carbon nanotubes in solution for drug delivery application

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An application for drug/gene delivery system is attracted in bio application of carbon nanotube research due to its unique structure. An encapsulation of medical agent and DNA into carbon nanotubes has reported so far. Also spatial distribution analysis of carbon nanotubes within an organism after dosing of nanotubes is performed in-vivo. We report the diffusional motion analysis of nanotubes in viscous solution which is regarded as quasi in-vivo. Diffusion constant is determined from sequential images of nanotube in solution which is observed under a dark field microscope. Diffusional motion of nanotubes is analyzed by three components, which parallel, perpendicular, and rotation to nanotube axis. As a result, a parallel per perpendicular ratio diffusion constant that the ratio is theoretically predicted two is increased in limited space. This implies that nanotubes diffuse parallel direction dominantly near the wall; a cell wall in organism. In addition, in the case of viscous solution, it is estimated that parallel and perpendicular diffusion is faster than the predicted theoretically. On the other hand, rotational diffusion constant matches the theory. Although we have not revealed the reason absolutely at this moment, we suppose that the faster diffusion of nanotube in viscous solution is explained by diffusion in slip condition that profile drag is negligible in molecular scale. Therefore nanotube based drug/gene delivery has a greater tendency to spread wider than the prediction and shows directional diffusion that depends on nanotube axis, which leads to assistance for the progression of the bio application of nanotube.

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### Adsorption of Adenine and Thymine on Single-Wall Carbon Nanotubes

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The adsorption of adenine and thymine on the surface of metallic single-wall carbon nanotubes has been studied using local density approximation within density functional theory .This paper reveals energies and equilibrium distances for various configurations which has been obtained after relaxation of the system. To study the adsorption phenomenon of adenine and thymine on SWNT the molecular bonds and angels before and after adsorption were calculated. Due to the interaction of π-orbitals of adenine-thymine and p-orbitals of SWNT.The study reveals that there is not significant changes due to adsorption in electronic structure of metallic nanotubes.The obtained results from these studies gives insight to investigate the interaction of DNA on surface of single- wall carbon nanotubes.

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### Exploring bio-functionalized CNTs and their interaction with cells using atomic force and fluorescence microscopy

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At present, the atomic force microscope (AFM) offers a unique solution to study biological specimens on the nanometer scale under (near-) physiological conditions without the need for rigorous sample preparation, staining or labelling. We expected new and significant bio-physical insights into the delivery process and transport mechanism of CNTs into cells employing the AFM. Here we give an overview for the application of AFM to characterize and assess CNT surface bio-functionalization. We present the new and emerging technique of simultaneous topographical and recognition (TREC) to directly visualize functionality of biomolecules attached to CNTs under physiological conditions. Moreover, we show how topographic AFM imaging can be used to study the binding of functionalized single walled carbon nanotubes (SWNT), double walled carbon nanotubes (DWNT) and multi walled carbon nanotubes (MWNT) to various relevant biological membranes, including nuclear membranes and cell surfaces. Present experiments involve the combination of fluorescence and atomic force microscopy to localize binding of functionalized carbon nanotubes to cell surfaces. These preliminary studies will facilitate the investigation of the binding of fluorescently labelled CNTs to the cell and their possible internalization in a time resolved manner. We show first results of uptake experiments, where we were able to trace individual carbon nanotubes internalized into living cells.

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### Carbon nanotubes as drug delivery systems: Material-related problems and how to solve them

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Aqueous dispersions of functionalized carbon nanotubes (CNTs) are widely used for biomedical applications, such as drug delivery, gene delivery, or cellular/in vivo imagining. The dispersion stability of such preparations, however, depends on a wide range of parameters, such as length, aspect ratio, surface charge, and functionalization of the nanotubes, as well as pH and composition of the surrounding medium. We have undertaken an extensive study to understand how these factors can be tuned in order to obtain an optimal dispersion stability of carbon nanotubes in chemical and biological environments. Furthermore, we have been able to demonstrate that a carbon nanotube-based delivery system for anticancer drugs loses its therapeutic efficacy, if the dispersion stability is poor. Another material-related problem for the use of oxidized carbon nanotubes as drug delivery systems is the generation of oxidation debris during the acid oxidation process. Previous studies have mainly focused on the characterisation of this debris and how to remove it, as it can present a pitfall for effective covalent functionalization of CNTs (which is likely to occur at the level of the debris and not the actual CNT surface). We went a step further and investigated the effect of present oxidation debris on the drug delivery properties of carbon nanotubes. Preliminary results indicate that oxidation debris has a much higher capability to transport drug molecules inside cancer cells than carbon nanotubes, comparable to oxidised graphene.

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### Synthesis of 14C-labelled Carbon Nanotubes for in vivo biodistribution studies

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Carbon nanotubes (CNT) are currently developed for multiple future commercial applications. It is therefore more than ever necessary to address their health safety implications and in particular explore their in vivo biodistribution and pharmacokinetics. One critical point for such investigation is the labelling strategy of CNT in order to track their behavior and fate in the body that could lead to some surface modifications influencing interactions of CNT with biological materials. In a first step we developed a new post treatment method that allows the 14C-labeling of purified MWCNT without modifying their structure. Results of a preliminary biodistribution study in rats will be presented. However, MWCNT produced through this method could not reach a sufficient 14C-labeling level for in vivo bio-persistence studies. In order to increase the specific activity of the 14C-labelled MWCNT we developed a process based on the previously reported aerosol-assisted CCVD process4. For the first time, MWCNT were synthesized by the direct use of 14C-labelled benzene as the carbon source and were fully characterized (SEM, TEM, TGA). Long and aligned CNT (controllable length around 100µm, mean external diameter of 40 nm) that are uniformly radiolabelled with a very high specific activity (more than 100 µCi/mg) have been formed. Thanks to the high specific activity of these 14CNT, low quantity (~1µg) of CNT will be used to contaminate a series of rats. Further in vivo experiments will be designed to evaluate the eventual bio-accumulation and bio-persistence of CNT.

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### Toxicology Study of Single-Wall Carbon Nanohorns with Different Sizes Intravenously Administrated in Mice

**Minfang Zhang**, *National Institute Of Advanced Industrial Science And Technology, Japan* | **Takashi Yamaguchi**, *Nagoya University* | **Sumio Iijima**, *National Institute Of Advanced Industrial Science And Technology, Japan; Nagoya University; Meijo University* | **Masako Yudasaka**, *National Institute Of Advanced Industrial Science And Technology, Japan*

With the study of carbon nanotubes on biomedical applications, their toxicity is a critical issue. It has been realized that the toxicity of nanotubes is related to their length and impurities. However, the knowledge on toxicity of carbon nanotubes is still limited. Herein, we have studied the immune toxicities and biodistribution of single-wall carbon nanohorns (SWNHs) which were intravenously administered in mice. We used SWNHs with two different aggregate-sizes: 80-120 nm and 30-50 nm. The latter ones were separated from the former ones by sucrose gradient centrifuge. The hematologic test showed that the blood counts and the differential counts of white blood cells did not show much difference between two types of SWNHs and control PBS. The measurements of proinflammatory cytokines revealed that there were no significant releases of TNF-ƒ¿, IFN-ƒÁ and IL-6 whatever samples were injected. The biodistribution of SWNHs were investigated by using Gd2O3 labeled SWNHs. The results showed that the blood circulation time of SWNHs with small sizes were longer (about 6 h) than that of SWNHs with larger sizes (<1 h). After 24 h since the administration, both of two sized SWNHs were mainly localized in liver and spleen, and significantly, a few of SWNHs (about 5%) existed in intestines. We also found trace amount of SWNHs in feces from one mouse, suggesting that SWNHs could be excreted from mouse.

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### Peek/Carbon Nanotube Composite Compatibilized with Polysulfones

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The structure, morphology, thermal and mechanical properties of high performance poly(ether ether ketone) (PEEK) based composites incorporating different single-walled carbon nanotubes (SWCNTs) and polysulfones as compatibilizers have been investigated. X-ray diffraction patterns of the SWCNTs dispersed in the polysulfones revealed an effective debundling and disentanglement of the nanotubes. Microscopic observations showed that wrapped SWCNTs were homogenously dispersed in PEEK using mechanochemical pre-treatments in ethanol followed by a melt-extrusion process. TGA thermograms demonstrated a remarkable increase in the degradation temperatures of the matrix by the addition of the SWCNTs, attributed to the compatibilizing effect and the high thermal stability of the polysulfones. The addition of very small amounts of wrapped SWCNTs raised the crystallization temperature of PEEK, whereas it decreased at higher concentrations, due to the inactive nucleating effect of the nanofillers, the restrictions on chain diffusion imposed by the nanotube network and the presence of an amorphous compatibilizer miscible with PEEK. The polysulfones increased the stiffness and toughness of the composites, attributed to an improved filler dispersion and stronger matrix-reinforcement interfacial adhesion. Improved properties were observed for composites incorporating the compatibilizer with higher structural similarity to the matrix. The overall performance of these composites is suitable for use in lightweight structural applications, particularly for the aeronautic industry.

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## Effect of Carbon Nanotube Diameter Distribution and Morphology on the Electrical Conductivity Properties of Polycarbonate Composite.

**Ricardo Prada Silvy**, *SouthWest NanoTechnologies, USA* | **Yongqiang Tan**, *SouthWest NanoTechnologies, USA* | **Alexander Down**, *SouthWest NanoTechnologies, USA* | **Robert Socher**, *Leibniz Institute of Polymer Research Dresden, Germany* | **Petra Pötschke**, *Leibniz Institute of Polymer Research Dresden, Germany*

SWCNT materials are difficult to disperse in melt compounds and are less commercially available than conventional MWCNT. MWCNT are preferred as a conductive additive for thermoplastic polymers. MWCNT, however, often results in mechanical properties being compromised when compared to the unfilled polymer. Therefore, new special CNT need to be developed for those polymer composites that require better electrical and mechanical performance than are currently possible from conventional MWCNT and do not have the dispersion problems associated with SWCNT. In this research, electrical conductivity of different composites consisting of several different MWCNT added to polycarbonate was investigated. The performance of few-walled CNTs having 3-6 walls (5-7 nm diameters) was compared with two commercial MWCNT having larger diameter and similar carbon purity. Melt mixing of polycarbonate Makrolon 2600 PC granules with MWCNT was carried out at 280°C using a DSM micro-compounder. Electrical conductivity measurements were performed using the ASTM D257 and ATSM D4496 methods on compression molded plates. The lowest electrical percolation threshold (0.25-0.38 wt% CNT loading) was found for the straight few-walled CNT material. Resistivity at 0.5-1.0 wt% CNT loading was between 104-102 Ohm cm. Percolation thresholds are between 0.38-0.50 wt% and 0.50-0.65 wt% for conventional MWCNT having average diameter between 7-9 nm and 12-15 nm, respectively. TEM analysis revealed noodle-type structure for the MWNT sample having 7-9 nm diameters. Few-walled, straight tubes having average diameter between 5-7 nm provide higher conductivity properties at lower loading levels than traditional MWCNT while reducing or eliminating adverse effects on mechanical properties.

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## Carbon Nanotube Thin Films: Flexible Substrates for the Assembly of Inorganic Nanomaterials

**Gregor Lawson**, *Department of Chemistry and the Brockhouse Institute for Materials Research, McMaster University, Canada* | **Parsian Mohseni**, *Department of Engineering Physics and the Center for Emerging Device Technologies, McMaster University* | **Ray Lapierre**, *Department of Engineering Physics and the Center for Emerging Device Technologies, McMaster University* | **Alex Adronov**, *Department of Chemistry and the Brockhouse Institute for Materials Research, McMaster University, Canada* | **Ryan Chadwick**, *Department of Chemistry and the Brockhouse Institute for Materials Research, McMaster University, Canada*

The deposition of inorganic nanoparticles upon the surface of carbon nanotubes has received much attention in recent years. Research within this field has been driven by the desire to develop new composite materials exhibiting novel electronic, optical, and catalytic properties. In addition to the decoration of individual nanotubes, several groups have investigated the use of CNT thin films as scaffolds for the assembly inorganic nanostructures and other secondary materials, such as polymers and biomaterials. Nanotube films exhibit a number of physical properties which make them suitable for such applications, displaying impressive electrical conductivity, flexibility, and thermal stability while also possessing a high surface area upon which chemical modification can be conducted. Here, we present work demonstrating the potential of carbon nanotube thin films as flexible conductive substrates for the support of a variety of inorganic nanostructures including Au nanoparticles and III-V semiconductor nanowires.[1, 2] Recent progress towards the development of functional electronic devices incorporating these novel composite materials will also be discussed. [1] Lawson, G.; Gonzaga, F.; Huang, J.; de Silveira, G.; Brook, M. A.; Adronov, A. J. Mater. Chem. 2008, 18, (14), 1694-1702. [2] Mohseni, P. K.; Lawson, G.; Couteau, C.; Weihs, G.; Adronov, A.; LaPierre, R. R. Nano Lett. 2008, 8, (11), 4075-4080.

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## Functionalization of SWCNT for incorporation into epoxy matrix. Processing conditions and sample formulation

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The one-dimensional structure of single walled carbon nanotubes (SWCNT), their low density, high aspect ratio, and extraordinary mechanical, electrical and thermal properties make them particularly attractive as reinforcements in multifunctional composite materials. A great challenge in SWCNT/polymer composites is the efficient translation of nanotube properties into the polymer matrix. A prerequisite for such an endeavour is an efficient dispersion of individual nanotubes and the establishment of a strong chemical affinity with the surrounding polymer matrix. Functionalized SWCNT have the potential to solve these problems. Through covalent chemistry on negatively charged SWCNT it is possible to attach different functionalities to the nanotube sidewall. In this work we have incorporated negatively charged SWCNT directly into a polymer precursor or after their functionalization with acid and amine functionalities on the nanotube sidewall. The functionalization of the SWCNT was characterized in detail. A commercial trifunctional epoxy resin used in the aerospace industry, triglycidyl p-amino phenol (TGAP), was used as the polymeric matrix precursor. Multifunctional resins such as TGAP posses a high crosslinking density which translates in a high modulus and strength however this also invariably leads to a brittle polymer. The mechanical performance of these epoxy/SWCNT composites was evaluated as well as the optimal processing conditions and changes in resin formulation necessary to achieve a significant enhancement in mechanical properties by incorporation of functionalized SWCNT. The highest improvement in toughness was achieved by direct integration of negatively charged SWCNT. Several spectroscopic techniques were used to characterize the SWCNT dispersion and interaction with the matrix.

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## Enhanced Electric Double Layer Capacitance of Poly Sodium 4-Styrensulfonate/Graphene Oxide Electrodes with High Cyclic Performance

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We have synthesized poly sodium 4-styrensulfonate intercalated graphite oxide and characterized its chemical and physical properties. We found that the interlayer distance of a PSS-treated graphite oxide increased by about 1 Angstrom compared to that of the precursor graphite oxide. This increase in interlayer spacing was attributed to the intercalation of a monolayer of planar PSS into the graphite oxide interlayers facilitated by a π-π interaction between the aromatic rings of the graphite oxide and PSS. The PSS-intercalated graphite oxide had a higher structural stability than the pristine graphite oxide during thermal treatment because of the high melting point of PSS, resulting in high specific capacitance (189.4 F/g), energy density (26.16 Wh/kg), and momentum density (90.68 W/kg) with high cyclic performance. We will discuss more detail in the talk.

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### Synthesis, Characterization and Photoelectronic Property of Carbon Nanotube-PbS Quantum Dot Nanohybrids

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Carbon nanotube (CNT)-semiconductor quantum dot (QD) nanohybrids are of great interest for the development of next generation photovoltaic (PV) devices. On one hand, the semiconductor QDs can serve as tunable light-harvesting assemblies through size quantization effect. On the other hand, the unique electrical and electronic properties, wide electrochemical stability window, and high surface area render CNTs as ideal scaffolds for anchoring light-harvesters and directing the flow of photogenerated charge carriers. Among the various semiconductor materials, PbS QDs have been attracting particular attention due to their narrow band gap (0.41 eV for bulk) and large excitonic Bohr radius (~18 nm). These specific advantages make PbS QDs applicable in the infrared range that comprises ~40% of the solar spectrum. More interestingly, the recent discovery of multiple exciton generation (MEG) effect in PbS QDs opens up the possibility of overcoming the ordinary thermodynamic limit of solar energy conversion. In this presentation, colloidal PbS QDs with a relatively monodispersed size distribution are synthesized and hybridized with both single-walled and multi-walled CNTs to construct CNT/PbS-QD nanohybrid architectures. Surface modifications on CNTs such as acid treatment and ligand decoration are performed to create functional sites for attaching PbS QDs. A variety of techniques such as Raman, FT-IR and XPS are employed to characterize the functionalized CNTs. The effect of surface modification of CNTs on the configuration (morphology, density and distribution of coupled QDs etc.) of CNT/PbS QD nanohybrids is studied by TEM. Furthermore, photoluminescence and photoelectronic properties of the CNT/PbS-QD nanohybrids are investigated systematically.

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### Novel Nanocomposites between Natural Rubber Latex and Iron-Filled Carbon Nanotubes: Preparation, Characterization, Electrical and Mechanical Properties

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The present study describes the preparation, characterization and study of electrical and mechanical properties of nanocomposites between of natural rubber latex (NR) and iron-filled multiwall carbon nanotubes (MWCNTs)[1]. Several samples have been prepared containing different amounts of MWCNTs (from 0.01 to 10 wt%) using the aqueous dispersion method[2]. The nanocomposites were characterized by X-ray micro-tomography, transmission (TEM) and scanning electron microscopy (SEM), force atomic microscopy (AFM), Raman and FT-IR spectroscopies, XRD and TGA/DSC, and the main results obtained through these techniques will be discussed. The quality of the CNTs dispersion into NR has been evaluated by microscopy and micro-tomography. The electrical resistivity of the samples showed a significant improvement in the conductivity with the MWCNT addition. For example, the resistivity varied from 109 (NR) to 103 Ω.cm-1 after the addition of 10 wt% of MWCNT. The percolation threshold concentration was found between 1-2wt.%. Significant improvements on the mechanical properties of nanocomposites were also observed. In comparison to the neat NR, increases of 250% in Young modulus and 720% in the tensile at break have been observed for the nanocomposite with 3.5 wt% of MWCNT. Due the presence of magnetic species encapsulated into MWCNT cavities, the nanocomposites present also magnetic behavior, resulting in novel kind of multifunctional materials with a great potential for further applications. ACKNOWLEDGMENTS: Brazilian network on CNT research, INCT-Nanocarbono, CNPq, CAPES-PROCAD. 1. M.C. Schinitzler, M.M. Oliveira, D.M. Ugarte,A.J.G. Zarbin, Chem. Phys. Lett., 381 (2003) 541. 2. L.F. Valadares, C.A.P. Leite, F. Galembeck, Polymer, 47 (2006) 672.

## Poster Board | 222

### Different CNT in PC/SAN blends containing a reactive component

**Maren Gültner**, *Leibniz Institute Of Polymer Research Dresden, Germany* | **Andreas Göldel** | **Petra Pötschke**

Systems of polycarbonate (PC), poly(styrene-co-acrylonitrile) (SAN), multi-walled carbon nanotubes (MWNT) functionalized with amino-groups (Nanocyl® 3152), MWNT (Nanocyl® 3150, 7000) or high-purity single-walled carbon nanotubes (SWNT, HipCo), and a reactive component (RC, N-phenylmaleimide styrene maleic anhydride) were melt mixed in a DSM Xplore microcompounder. The RC is miscible with SAN and contains maleic anhydride groups which have the potential to couple reactively with the functionalized MWNT. The influence of the RC on the localization of MWNT and SWNT and the electrical resistivity of the MWNT filled blend systems of PC and SAN was investigated. In PC/SAN blends without the RC the MWNT are localized in the PC phase. However, in SAN modified by RC the functionalized MWNT localize in the SAN-RC phase. The localization of the MWNT after addition of the RC depends on the concentration of the MWNT and the RC. By adapting that ratio and the mixing strategy, the localization of the multiwalled carbon nanotubes can be tuned. The high-purity SWNT behave differently compared to the MWNT. Using 0.5 wt% SWNT and a amount of 5 wt% RC the SWNT localize in PC, whereas MWNT were found at these concentrations in SAN. The investigations have shown that carbon nanotubes (CNT) once coupled with the RC localize in the SAN-RC Phase. Thus, the chemical reaction and/or strong interactions seem to be the driving forces for the localization of MWNT in SAN-RC.

## Poster Board | 225

### The key parameters for alignment of carbon nanotubes by wet electrospining

**Milana Lisunova**, *Freie Universitat Berlin, Fachbereich Physik, Germany* | **Vitaliy Datsyuk** | **Stephanie Reich** | **Attila Hildmann** | **Benjamin Hatting**

The key parameters for alignment of carbon nanotubes by wet electrospining Milana Lisunova, Attila Hildmann, Benjamin Hatting, Vitaliy Datsyuk, Stephanie Reich Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany A promising application within the near future are CNTs as nanoscale fillers in composite materials with attractive conductivity- and tensile strength. In many important applications CNTs can realize their full potential only if they are aligned, and their entangled agglomerates are destroyed. For example, electrical and thermal conductivities of aligned CNTs are higher than for the system with dispersed CNTs. Alignment of CNTs can be achieved by flow-induced alignment, by applying magnetic and electrical fields and by electrospinning. Electrospinning is very promising for the alignment of CNTs because it can be used in mass production. The degree of alignment of carbon nanotubes with different surface morphology in electrospun nanofibers were investigated by polarized Raman spectroscopy and transmission electron microscopy (TEM). The influence of polymeric interface, such as cellulose acetate (CA), polyethylene oxide/polyvinyledene (PEO/PVP), polyacrylonitrile (PAN), polyimide resins (PP) on the alignment was studied by computer simulation and Raman spectroscopy. The highest level of ordering was found in lyotropic cellulose acetate liquid crystal nanofibers. We measured how the alignment of carbon nanotubes affects the thermal stability and activation energy of degradation of polymeric fibers.

## Poster Board | 228

### Aligned Carbon Nanotubes from Natural Materials

**Meng-Qiang Zhao**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology, China* | **Qiang Zhang**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology, China* | **Jia-Qi Huang**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology, China* | **Jing-Qi Nie**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology, China* | **Fei Wei**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology, China*

Many kinds of natural materials have been explored to lower the cost of raw materials during the mass production of carbon nanotubes (CNTs).[1] However, most of the as-obtained CNTs are always entangled with each other, and the mass production of aligned CNTs with low cost is still a challenge. Natural materials that can provide plane surfaces can be used as catalyst support for the synthesis of aligned CNTs. Aligned CNTs were intercalatedly produced among the layered materials (e.g. mica, vermiculite),[2] and a yield of 3.0 kg/h were achieved in fluidized bed reactor.[3] Besides, wollastonite were also used for the production of aligned CNTs,[4] leading to the formation of leaf-like and brush-like wollastonite/CNT hybrids. To further reduce the production cost, liquid petroleum gas (LPG) were explored as carbon source for the production of aligned CNTs on the above mentioned natural materials. Moreover, long aligned CNTs were successfully obtained from LPG on quartz flake or spheres.[5]. This provides a series of aligned CNTs from natural materials with unique structure and properties that can be produced at a low cost, and used as fillers, or energy-absorbing materials. [1] D. S. Su, ChemSusChem 2009. [2] Q. Zhang, et al, Advanced Materials 2009. [3] (a) Q. Zhang, et al, Carbon 2009; (b) Q. Zhang, et al, Carbon 2010. [4] M. Q. Zhao, et al, ChemSusChem 2010. [5] (a) J. Q. Huang et al, Carbon 2008; (b) Q. Zhang, et al, Chinese Science Bulletin 2007.

## Poster Board | 231

### Preparation of silica gel microparticles homogeneously coated by pristine carbon nanotubes for the HPLC stationary phase

**JongTae Yoo**, *Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Japan* | **Tsuyohiko Fujigaya**, *Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Japan* | **Naotoshi Nakashima**, *Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, Japan; Japan Science and Technology Agency, CREST*

Carbon nanotubes (CNTs) have unique ƒÎ-rich, hydrophobic and curvature surfaces. Interfacial interactions of CNTs with molecules have been the focus of interests in the aspect from solubilization of CNTs through physisorption and many applications. However, no systematic investigations for the degree of interactions have been carried out due the lack of evaluation methodology. In this situation, the chromatography-based analysis using CNTs as a stationary phase provides precise as well as higher throughput method. We succeeded the first non-covalent coating of the silica gel with pristine single-walled carbon nanotubes (SWNTs) (denote as SWNT/NH2-silica) and the utilization of the gel for liquid chromatography stationary phase. The present method is extremely simple and efficient with neglectable damage on SWNT intrinsic structure and offers a morphologically controlled coating on silica gel by SWNTs. And this method permit homogeneous wrapping of selected SWNTs, so analysis interaction of target SWNTs with molecules. We fabricated the HPLC column packed with the SWNT/NH2-silica (denote as SWNT/NH2 -column) and NH2-silica (denote as NH2-column) as well. SWNT/NH2-column gave different retention time from that of NH2-column for the same solute, which clearly indicate SWNTs on the gel served as an affinity-based stationary phase. And we verified separation of benzene groups by retention time. This separation has roots in different interaction of SWNTs with benzene groups. We believe that SWNT/NH2-column provide the promising opportunity for the systematic studies using wide range of molecules to achieve the deep understanding of the degree of interaction between CNTs and molecules.

## Poster Board | 234

### Ceramic Nanocomposites with Conventional and Doped Carbon Nanotubes as Fillers

**Frank Dillon**, *Department of Materials, Oxford University, United Kingdom* | **Antal Koos**, *Department of Materials, Oxford University, United Kingdom* | **Geoffrey Otineo**, *Department of Materials, Oxford University, United Kingdom* | **Richard Todd**, *Department of Materials, Oxford University, United Kingdom* | **Nicole Grobert**, *Department of Materials, Oxford University, United Kingdom*

Incorporation of carbon nanotubes (CNT's) into appropriate matrices can result in composite materials which are expected to have enhanced mechanical, thermal and electrical properties. The combination of nanotubes with a ceramic matrix could potentially create composites that have high-temperature stability as well as exceptional toughness and creep resistance. However, achieving a homogeneous dispersion of tubes in an oxide material with strong bonding between tubes and matrix presents rather more of a challenge than incorporating tubes into a polymer matrix. Any practical applications of CNTs nanotubes necessitate fairly large amounts of material at commercially viable prices. Aerosol CVD appears to be the most suitable synthesis method for industrial scale production of CNTs. It is suitable for the continuous injection of catalyst precursor and carbon feedstock, requires no additional catalyst preparation step and the samples need minimal or no purification. This work focuses on using a silica ceramic called mesoporous silica as a matrix material for conventional and doped carbon nanotubes. We describe a process where pre-prepared CNTs are mixed with the synthesis gel of mesoporous silica to prepare the nanocomposite. This is achieved by adjusting the surface chemistry of the CNTs so an improved interface interaction with the silica matrix is achieved. The incorporated nanotubes were uniformly dispersed throughout the powders and that a strong interface between the tubes and matrix was formed. The powder samples were then pressed and fired to prepare dense samples for thermal conductivity and mechanical testing.

## Poster Board | 237

### Synthesis, Characterization, and Physical Properties of Europium-Nanowires Encapsulated in Single Wall Carbon Nanotubes

**Ryo Nakanishi**, *Department of Chemistry, Nagoya University, Japan* | **Ryo Kitaura**, *Department of Chemistry, Nagoya University, Japan* | **Hidetsugu Shiozawa**, *Advanced Technology Institute, University of Surrey, United Kingdom* | **Paola Ayala**, *Faculty of Physics, University of Vienna, Austria* | **Katrien DeBlauwe**, *Faculty of Physics, University of Vienna, Austria* | **Christian Kramberger-Kaplan**, *Faculty of Physics, University of Vienna, Austria* | **Takeshi Saito**, *Nanotechnology Research Institute, AIST, Japan* | **Choi Daeheon**, *Department of Chemistry, Nagoya University, Japan* | **Yasumitsu Miyata**, *Department of Chemistry, Nagoya University, Japan* | **Hirofumi Yoshikawa**, *Department of Chemistry, Nagoya University, Japan* | **Kunio Awaga**, *Department of Chemistry, Nagoya University, Japan* | **Thomas Pichler**, *Faculty of Physics, University of Vienna, Austria* | **Hisanori Shinohara**, *Department of Chemistry, Nagoya University, Japan*

The chemically and thermally stable one-dimensional (1D) nano space of carbon nanotubes (CNTs) can be used as a nano-sized reaction vessel to fabricate novel low-dimensional nanomaterials such as nanowires. Fabrications of low-dimensional nanomaterials using CNTs are emerging on metal complexes, metal salts and molecules but still very few on metal nanowires, where we can expect interesting transport and magnetic properties arising from quantum effects. In this workCwe have successfully fabricate Eu nanowires, whose diameter ranges from one-atom thick to 4 rows of atoms, using 1D space of single wall CNTs and double wall CNTs. Formation of Eu nanowires was confirmed by High-resolution transmission electron microscopy (HRTEM), and their electronic structure was investigated by X-ray photoelectron spectroscopy (XPS). Cap-opened CNTs and Eu powder were sealed in Pyrex glass under high vacuum, and heated at 873 K for 2 days. Eu atoms attached at outer surface of CNTs were removed by HCl washing. Based on HRTEM images, filling ratio of Eu is estimated to be about 80 %. HRTEM images shows that structure of Eu nanowires strongly depend on the diameter of CNTs and distinctly different from that of bulk crystals. Some unique properties due to the 1D structure can also be observed from some measurement, for example SQUID, XPS and so on, so we want to discuss about them.

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### Synthesis and Characterization of Single-walled Carbon Nanotubes -Alumina Nanocomposites

**Fernando Machado Machado**, *Universidade Federal Do Rio Grande Do Sul, Brazil* | **Mônica Jung De Andrade**, *Universidade Federal Do Rio Grande Do Sul, Brazil* | **Carlos Pérez Bergmann**, *Universidade Federal Do Rio Grande Do Sul, Brazil* | **Solange Binotto Fagan**, *Centro Universitário Franciscano*

Carbon nanotubes have been investigated extensively over the past decade for adsorption and sensors applications. This paper reports the synthesis and characterization of single-walled carbon nanotubes (SWCNT)-alumina nanocomposites. SWCNTs (mean diameter of 1,63 nm) were produced by catalytic chemical vapor deposition for the preparation of such nanocomposites. To obtain a good dispersion of SWCNTs in the alumina matrix, they were functionalized by: one covalent (with nitric, sulfuric and chloridric acids) and two non-covalent (with polyvinyl alcohol, PVA, and sodium dodecyl sulfate, SDS) functionalizations. Nanocomposites were prepared by chemical precipitation using Al(NO3)3.9H2O and NH3.H2O as starting material for Al2O3. Then, these composites were submitted to a thermal treatment at 500°C for 2h in argon atmosphere. Structural defects on SWCNTs and the resulting interaction between matrix and the SWCNTs were verified by Raman spectroscopy. To study the microstructure of these nanocomposites specific surface area (BET), scanning (SEM) and transmission (TEM) electron microscopy were carried out, while X-ray diffraction (XRD) was used to verify the crystallization of alumina. The surface area of the resulting nanocomposites reached 265.90 m2/g for covalently functionalized ones, 280.80m2/g and 211.52 m2/g for the non covalently functionalized with PVA and SDS, respectively. XRD confirmed crystallization of gamma-alumina. The preeminent properties of the SWCNTs-Al2O3 nanocomposite powders might be interesting to use as adsorbents devices (for example, fluoride from water) due to high surface area and interface reactive properties.

References: [1] Y. Li, S. Wang, A. Cao, D. Zhao, X. Zhang, et al.; Chemical Physics Letters n.350, p. 412–416, 2001. [2] B. Gómez and J.M. Martínez-Magadán; J. Phys. Chem, n.109, 2005. [3] J. Goering and U. Burghaus; Chemical Physics Letters n.447, p. 121–126, 2007 [4] M.D. Lima, M.J de Andrade, A. Locatteli, et al.; Physica Status Solidi b-Basic Solid State Physics, v. 244, p. 3901-3906, 2007. [5] M.J de Andrade, A. Weibel, C. Laurent, et al., Scripta Materialia, v. 61, p.988-991, 2009. [6] Q. Yang, Y. Deng, and W. Hu; Ceramics International n.35, p. 1305–1310, 2009.

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# Tuesday, June 29

## 15:33-17:00 Poster Session 2

### Poster Board | 2

### Raman and Electrical Properties of Artificial Bilayer Graphene

**Hoyeol Yun**, *Konkuk University* | **Youngwook Kim**, *Pohang University of Science and Technology* | **Unseok Jung**, *Konkuk University* | **Seung-Geol Nam**, *Pohang University of Science and Technology* | **Dongchul Kim**, *Samsung Advanced Institute of Technology* | **Sunea Seo**, *Samsung Advanced Institute of Technology* | **Hu-Jong Lee**, *Pohang University of Science and Technology* | **Junsung Kim**, *Pohang University of Science and Technology* | **Sang Wook Lee**, *Konkuk University*

Raman and electric transport properties of the artificial bilayer graphene were investigated. The position of single layer graphene flake can be controlled thanks to the transfer contact printing technique. Two different graphene samples were prepared by mechanical exfoliation and partially stacked one on the other using PMMA as a graphene carrier and measured its optical and electrical properties. In contrast to the regular Bernal stacking of bilayer graphene, two layers of the artificial bilayer graphene are arbitrarily misoriented. Such a misorientation has been predicted to decouple the two graphene sheets. Due to the broken AB stacking, bilayer stack shows almost identical Raman spectrum while its 2D band is being shifted to its right, indicating the reduction of Fermi velocity. The coupling between the graphene layers is examined by the interlayer transport measurements.

### Poster Board | 5

### A Controllable Self-Assembly Method for Large-Scale Synthesis of Graphene Sponges and Free-Standing Graphene Films

**Fei Liu**, *KAIST* | **Tae SeokSeo**, *KAIST*

Here we present a simple method to prepare large-scale graphene sponges and free-standing graphene films using a speed vacuum concentrator. During a centrifugal evaporation process, suspended graphene oxide (GO) sheets in an aqueous solution have been assembled to generate network-linked GO sponges or a series of multilayer GO films depending on the temperature of a centrifugal vacuum chamber. While sponge-like bulk GO materials (GO sponges) have been produced at 40°C, uniform free-standing GO films which size were up to 9 cm^2 were generated at 80°C. The thickness of GO films can be controlled from 200 nm to 1 um based on the concentration of the GO colloidal suspension and evaporation temperature. The synthesized GO films exhibit excellent transparency, typical fluorescent emission signal and high flexibility with a smooth surface and condensed density. Reduced GO sponges and films have been produced with less than 5 wt% content of oxygen through thermal annealing process at 800°C with H2/Ar flow. A structural flexibility of the reduced GO sponges which have highly porous, interconnected and three-dimensional network, and excellent electrochemical properties of the reduced GO film with respect to electrode kinetics for the [Fe(CN)6]3-/4- redox system have been demonstrated.

### Poster Board | 8

### Stress distribution in a deformed graphene monolayer nanocomposite

**Lei Gong**, *School of Materials, University of Manchester* | **Ian Kinloch**, *School of Materials, University of Manchester* | **Robert Young**, *School of Materials, University of Manchester* | **Kostya Novoselov**, *School of Physics and Astronomy, University of Manchester*

Graphene is one of the stiffest known materials, with a Young's modulus of 1 TPa, making it an ideal candidate for use as a reinforcement in high-performance composites. However, being a one-atom thick crystalline material, graphene poses several fundamental questions: (1) can decades of research on carbon-based composites be applied to such an ultimately-thin crystalline material? (2) is continuum mechanics used traditionally with composites still valid at the atomic level? (3) how does the matrix interact with the graphene crystals and what kind of theoretical description is appropriate? We have demonstrated unambiguously using Raman Spectroscopy that stress transfer takes place from the polymer matrix to monolayer graphene in a composite, showing that the graphene acts as a reinforcing phase. We have also modelled the behaviour using shear-lag theory, showing that graphene monolayer nanocomposites can be analysed using continuum mechanics. Additionally, we have been able to map the distribution of stress in the graphene monolayer. It is found that the stress is distributed uniformly in the centre of the monolayer and falls to a low level at the edges. There are also some regions where the stress is low which may be attributed to the geometry of the graphene monolayer, where it is not completely flat.

### Poster Board | 11

### New graphene and few layer graphene (FLG) synthesis methods and their catalytic applications

**Izabela Janowska**, *Laboratoire des Matériaux, Surface et Procédés pour la catalyse (LMSPC), France* | **Ovidiu Ersen**, *Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS) UMR 7504 CNRS, France* | **Kambiz Chizari**, *Laboratoire des Matériaux, Surface et Procédés pour la catalyse (LMSPC), France* | **Spyridon Zafeiratos**, *Laboratoire des Matériaux, Surface et Procédés pour la catalyse (LMSPC), France* | **Victor Da Costa**, *Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS) UMR 7504 CNRS, France* | **Dominique Bégin**, *Laboratoire des Matériaux, Surface et Procédés pour la catalyse (LMSPC), France* | **Marc-Jacques Ledoux**, *Laboratoire des Matériaux, Surface et Procédés pour la catalyse (LMSPC), France* | **Cuong Pham-Huu**, *Laboratoire des Matériaux, Surface et Procédés pour la catalyse (LMSPC), France*

Three new different synthesis methods of graphene and few layer graphene like (FLG) materials were developed. Two of them were based on the use of the microwaves irradiation, the first one: to induce the catalytic unzipping of the carbon nanotubes and an exfoliation of the expanded graphite in the second one [1, 2]. The last method, very recently developed, was based on the use of the mechanical thinning of graphite. All methods have different advantages: unzipping of the carbon nanotubes allows the control of the number of the graphene sheets in the final products, the FLG obtained from the expanded graphite consist of big size (up to few tenth micrometers) sheets and finally the third method results in high yield (up to 60%), low cost and process simplicity which make it very promising for the industrial scale applications. The obtained graphene and FLG were characterized by different microscopic and spectroscopic techniques such as TEM, TEM-SAED, TEM-DF-SAED AFM, XPS, IR. The results obtained from catalytic application of the graphene/FLG supported palladium catalyst, in the selective hydrogenation of cinnamaldehyde, will be compared with the ones from the Pd/CNTs use. 1. I. Janowska, O. Ersen, T. Jacob, P. Vennégues, D. Bégin, M.-J. Ledoux, C. Pham-Huu, App. Catal. A, 2009, 371, 22. 2. I. Janowska, K. Chizari, O. Ersen, S. Zafeiratos, D. Soubane, V. Da Costa, V. Speisser, Ch. Boeglin, M. Houllé, D. Bégin, D. Plee, M.-J. Ledoux, C. Pham-Huu, Nano Research 2010, 3, 126.

### Poster Board | 14

### Work Function Controlled Graphene Electrode for electron havesting device

**Hyeon Jin Shin**, *Samsung Electronics, LTD., SAIT; Sungkyunkwan University* | **Dukhyun Choi**, *Samsung Electronics, LTD., SAIT* | **WonMook Choi**, *Samsung Electronics, LTD., SAIT* | **Han**, *Sungkyunkwan University* | **Young Hee Lee**, *Sungkyunkwan University* | **Jae-Young Choi**, *Samsung Electronics, LTD., SAIT*

Recently, graphene has attracted enormous scientific attention on account of its extraordinary electronic and mechanical properties resulting from its one-atom-thick layers and hexagonally arranged sp2-hybridized carbon atom structure. The single graphene layer is a semimetal or zero-gap semiconductor, and has excellent electronic properties, for instance, high mobility (15000 cm2V-1s-1) and room-temperature quantum Hall effect. These superb characteristics of graphene open a new possibility of application in many electronic devices. In particular, to apply for p-n diode such as nanogenerator, the graphene layer need to matching of band diagram with next layer to improve efficiency of electron and hole transfer. To complete the integrated graphene-based nanogenerator, we need to control the work function of graphene. In this paper, we report on the first try to control the work function of growth graphene by diverse chemical doping from 4.0 to 5.0. Furthermore, we observed working behaviors of electron according to graphene electrode having a diverse work function in energy harvesting device such as nanogenerator. Our results suggest, therefore, work function controlled graphene are suitable for replacement of several novel metals.

## Poster Board | 17

### Dynamic superlubricity of graphene flake on graphite surface

**Irina Lebedeva**, *Moscow Institute of Physics and Technology, Russia; RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Moscow, Russia* | **Andrey Knizhnik**, *RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Moscow, Russia* | **Andrey Popov**, *Institute of Spectroscopy, Russia* | **Olga Ershova**, *Moscow Institute of Physics and Technology, Russia* | **Yurii Lozovik**, *Institute of Spectroscopy, Russia* | **Boris Potapkin**, *RRC Kurchatov Institute, Moscow, Russia; Kintech Lab Ltd, Moscow, Russia*

Different mechanisms of diffusion and drift of a graphene flake on a graphite surface are systematically analyzed using ab initio calculations and calculations with empirical potentials. A new mechanism of diffusion, "dynamic superlubricity", is proposed. According to the proposed mechanism, rotational transition of the flake to incommensurate states takes place with subsequent simultaneous rotation and translational motion until the commensurate state is reached again, and so on. Due to the significant barrier for rotation of the flake, these events are rare. However, this factor is compensated by long distances passed by the flake before it returns to the commensurate state. The molecular dynamics simulations demonstrate that the proposed diffusion mechanism can be dominant under certain conditions. According to analytic expressions derived for the diffusion coefficient and mobility of the flake, the relative contribution of rotation to incommensurate states should be the most significant at temperature associated with the barrier for transition of the flake between adjacent energy minima in the commensurate state and should correspond to an increase of the diffusion coefficient by more than an order of magnitude. The results obtained can be also useful for study of dynamics of polyaromatic molecules on a graphite surface and should be qualitatively valid for a set of commensurate adsorbate-adsorbent systems. The methods of control over the diffusion and drift of graphene components in nanoelectromechanical systems are discussed. Moreover, the possibility to experimentally measure the barriers to relative motion of graphene layers by study of a graphene flake diffusion is considered.

## Poster Board | 20

### Low molecular density of single molecular magnet grafted on graphene and nanotubes

**Manuel Lopes**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France* | **Matias Urdampilleta**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France* | **Andrea Candini**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France; CNR-INFM S3 research center, Italy* | **Antoine Reserbat-Plantey**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France* | **Laëtitia Marty**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France* | **Svetlana Klyatskaya**, *Karlsruhe Institute of Technology, Karlsruhe, Germany* | **Mario Ruben**, *Karlsruhe Institute of Technology, Karlsruhe, Germany* | **Marco Affronte**, *CNR-INFM S3 research center, Italy* | **Nedjma Bendiab**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France* | **Wolfgang Wernsdorfer**, *Institut Néel, CNRS-UJF-INPG, Grenoble, France*

Graphene and carbon nanotubes are considered promising materials for applications in future molecular electronics. Particular interest lies in the field of molecular spintronics: molecular magnets exhibit exciting properties for spin manipulation however they are difficult to address individually. We propose to probe them by using carbon based devices as sensors [1]. One of the main challenges is to understand and control the deposition process and the grafting mechanism down to the molecular level. We present here our first studies on the grafting and the arrangement of single molecular magnets (TbPc2) [2] on graphene sheets for different number of layers. By means of micro-Raman spectroscopy and Atomic Force Microscopy, we demonstrated that the coupling interaction between the two materials is carried mainly by the Pi-systems. We found that the molecules selectively graft on graphene with uniform dispersion and a number of layers dependent density. Moreover, as the interaction is soft, the intrinsic electronics properties of graphene are preserved [3]. This work shows the possibility to build graphene-based devices with new magnetic functionalities for spintronics applications. References [1] L. Bogani and W. Wernsdorfer, Nature Mat., 2008, 7, 179. [2] S. Klyatskaya et al., J. Am. Chem. Soc., 2009, 131, 15143. [3] M. Lopes et al., in preparation.

## Poster Board | 23

### Fabrication and optical visibility of graphene flakes on SiO2 subtrates

**Hsuan-De Li**, *Chung Yuan Christian University* | **Yi-De Li**, *Chung Yuan Christian University* | **Jyun-Hong Chen**, *Chung Yuan Christian University* | **Yuan-Liang Zhong**, *Chung Yuan Christian University* | **Zhen-Yu Juang**, *National Tsing Hua University* | **Ke-Chiang Liu**, *National Tsing Hua University* | **Cii-Dong Chen**, *Academia Sinica*

Graphene has emerged as an exciting material because of the novel properties associated with its two-dimensional honeycomb structures. We have fabricated the graphene flakes by tape cleavage method and thermal chemical vapor deposition (CVD) synthesis. The first method is the cleavage of graphite with 3M scotch-tape to produce the graphenes in controlled environment under low temperature and humidity. The second method is by using a gas mixture of methane/hydrogen to synthesize the graphenes by copper foil, and the graphene of few layers are grown on copper surface and then transferred onto SiO2 substrate by FeCl3 solution. By the optical microscope to find graphene, we have developed a quick method to distinguish the thickness of graphene flakes. The distinguishable image of graphene can be taken by the color light on the optimal thickness of SiO2 layer calculated from reflection spectrum. The number of layer in graphene has been determined more precisely by analyzing the Raman spectrum and the image of atomic force microscope (AFM).

## Poster Board | 29

### Metallic-to-insulating transition in disordered graphene monolayers

**Michael Hilke**, *McGill University*

We show that when graphene monolayers are disordered, the conductance exhibits a metallic-to-insulating transition, which opens the door to new electronic devices. The transition can be observed by driving the density or Fermi energy through the mobility edge. At the Dirac point the system is localized, whereas at higher densities there is a region of metallic behavior before the system becomes insulating again at higher densities. The region of metallic behavior depends on the disorder strength and eventually vanishes at high disorder. This result is quite unexpected since in square lattices, scaling theory predicts that this metallic region does not exist in two dimensions, in contrast to graphene, where the lattice is a honeycomb.

## Poster Board | 32

### Electron irradiation effects on the dynamics of graphene bilayers

**Eduardo Cruz-Silva**, *Oak Ridge National Lab* | **Zachary M. Barnett**, *Oak Ridge National Lab* | **Andres Botello-Mendez**, *Oak*

*Ridge National Lab* | **Humberto Terrones**, *Oak Ridge National Lab* | **Mauricio Terrones**, *Oak Ridge National Lab* | **Bobby G. Sumpter**, *Oak Ridge National Lab* | **Vincent Meunier**, *Oak Ridge National Lab*

Graphene is a promising material for nanoelectronic devices, but in order to have a better control of its electronic properties it is crucial to have control of its thickness and edge shape. Recent methods have been proposed to this end, such as electron irradiation to exfoliate multilayered graphene, as well as Joule heating to have a controlled edge reconstruction; which present the advantage of being scalable. However, effects such as bilayer edge loop formation have been observed in most cases when graphene is annealed, and seem incompatible with controlled edge formation. Using quantum density functional theory we explore how electron irradiation effects the dynamics of graphene bilayers. Our results show that irradiation induced defects are responsible of modifying the edge dynamics and provide a new method for tailoring graphene atomic structure at the nanoscale.

## Poster Board | 35

### Optical Measurement of the Phase-Breaking Length in Graphene

**Luiz Gustavo Cançado**, *Universidade Federal de Minas Gerais* | **Ryan Beams**, *University Of Rochester* | **Lukas Novotny**, *University Of Rochester*

We experimentally determined the phase-breaking length of the conduction electrons in single layer graphene through confocal Raman spectroscopy. The phase-breaking length was extracted from the D band susceptibility at an edge by using the double-resonance model. By measuring the excitation point-spread function and utilizing prior knowledge of the sample's geometry, we determined the spatial variation of the Raman susceptibilities, which allowed us to extract the phase-breaking length and found it to be localized to less than 40 nm at the graphene edge.

## Poster Board | 38

### The Raman scattering efficiency of Graphene

**C. Casiraghi**, *Freie Universität Berlin* | **Ph. Klar**, *Freie Universität Berlin* | **E. Lidorikis**, *Universiti of Ioannina, Greece* | **R. Panknin**, *Freie Universität Berlin* | **A. C. Ferrari**, *Cambridge University (UK)* | **S. Reich**, *Freie Universität Berlin*

We determine the Raman scattering efficiency of graphene by measuring the G peak intensity, I(G), by sample substitution [1]. Two substrates are used: silicon covered with 300 nm oxide (Si/SiOx) and calcium fluoride (CaF2). On Si/SiOx, I(G) shows a strong dependence on excitation. This is due to substrate interference effects. On CaF2 the G peak intensity is smaller than on Si/SiOx, with no significant dependence on the excitation wavelength. We evaluate the absolute Raman efficiencies by comparison with the 322 cm-1 phonon intensity of CaF2 and by correcting the intensities with respect to the optical constants and spectrometer sensitivity. From the G peak intensity measured at 2.41 eV on CaF2, we get a Raman efficiency of about 240 x 10-5 m-1 Sr-1, which is 40 times bigger than the first order diamond peak efficiency, in agreement with previous measurements on graphite [2]. 1. J. M. Calleja, J. Juhl, M. Cardona, 17, 876 (1978) 2. N. Wada, S. A. Solin, Physica 105B, 353 (1981)

## Poster Board | 41

### Optical properties of graphene quantum dots with fractionally filled degenerate shell of zero energy states

**Devrim Guclu**, *National Research Council Of Canada* | **Pawel Hawrylak**, *National Research Council Of Canada*

Graphene quantum dots are atomically thick nanometer-scale islands etched out of a single graphene sheet. In this work, we focus on magnetic and optical properties of triangular dots with zig-zag edges. Strikingly, such structures were suggested[1] to lead to a magnetized band of degenerate zero-energy states at the Fermi level. In our recent works, an analytical derivation of the zero-energy states were obtained[2], and the ground state magnetic properties of the degenerate band was explored[3] showing a complete depolarization of the magnetized neutral shell as a new electron is added. In this work, we present new theoretical results describing the optical properties of triangular graphene quantum dots as a function of carrier density. The excitonic absorption spectrum as a function of shell filling is studied using exact diagonalization techniques. Photons can be absorbed by promoting electrons either (i) from the valence band towards the degenerate shell and conduction band, (ii) within the degenerate shell, or (iii) from the degenerate shell towards the conduction band, giving rise to a rich structure of absorption spectrum. We find that excitonic spectrum depends strongly on the filling fraction of the degenerate shell. Our new results show the importance of magnetization and correlations on the optical properties in triangular graphene quantum dots. [1] Fernandez-Rossier J. and Palacios J.J. 2007 Phys.Rev.Lett. 99 177204 [2] Potasz P., Güçlü A D, and Hawrylak P. 2010 Phys.Rev.B 81 033403 [3] Güçlü A D. Potasz P., Voznyy O., Korkusinski M, and Hawrylak P. 2009 Phys.Rev.Lett. 103 246805

## Poster Board | 47

### Formation of Atomic Carbon Chains from Graphene Nanoribbons

**Edwin Hobi Jr**, *Institute of Physics - University of Sao Paulo, Brazil* | **Renato B. Pontes**, *Institute of Physics - University of Sao Paulo, Brazil* | **Adalberto Fazzio**, *Institute of Physics - University of Sao Paulo, Brazil* | **Antônio J. R. da Silva**, *Institute of Physics - University of Sao Paulo, Brazil; Brazilian Synchrotron Light Laboratory, Brazil*

The formation of one-dimensional carbon chains from graphene nanoribbons is investigated using ab initio molecular dynamics. We show under what conditions it is possible to obtain a linear atomic chain via pulling of the graphene nanoribbons. The presence of dimers composed of two-coordinated carbon atoms at the edge of the ribbons is necessary for the formation of the linear chains, otherwise there is simply the full rupture of the structure. The presence of Stone-Wales defects close to these dimers may lead to the formation of longer chains. The local atomic configuration of the suspended atoms indicates the formation of single and triple bonds, which is a characteristic of polyynes.

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### DNA-decorated graphene chemical sensors

**Brett Goldsmith**, *University Of Pennsylvania* | **Ye Lu**, *University Of Pennsylvania* | **Nicholas Kybert**, *University Of Warwick* | **A.T. Charlie Johnson**, *University Of Pennsylvania*

We measure the sensing response of DNA functionalized graphene to various analytes. Graphene is the current flagship nanomaterial and has been actively studied as a chemical sensor since shortly after it was isolated. Increasingly sophisticated device processing has revealed that some early measurements of graphene chemical sensing have been amplified by unintentional functionalization. We start with chemically clean graphene transistors and purposefully functionalize them to allow chemical sensing responses not found using pristine graphene. By using different DNA sequences during our functionalization, we are able to change the chemical sensitivity of the graphene. The resulting devices show fast response times, complete recovery at room temperature and discrimination between several similar analytes. This work has been supported by the IC Postdoc program, REU and the Nano/Bio Interface Center.

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### Graphene Nanoribbon Materials

**Javier Carretero-Gonzalez**, *The AlanG. MacDiarmid Nanotech Institute* | **Elizabeth Castillo-Martinez**, *The AlanG. MacDiarmid Nanotech Institute* | **Ray Baughman**, *The AlanG. MacDiarmid Nanotech Institute*

In this work we have investigated the chemical and physical properties of assemblies of graphene nanoribbons. Like in the last century when the appearance of ladder or stranded polymers1 with graphitic structure became promising for high performance non-metallic materials, the recent synthesis of narrow graphene nanoribbons2 using various techniques enables exciting possibilities for developing multifunctional materials based on graphene ribbons that exhibit useful properties. The physical properties and applications possibilities of such materials will be described. References: 1.-S. A. Hurley, Prabir K. Dutt and C. S. Marvel, "New Thermally Stable Polymer with a Graphite-Type Structure", Journal of Polymer Science: Part A-1, Vol. 10, 1243-1261, 1972. 2.- Liying Jiao, Li Zhang, Xinran Wang, Georgi Diankov and Hongjie Dai, "Narrow graphene nanoribbons from carbon nanotubes", Nature, Vol. 458, 877-880, 2009.

## Poster Board | 59

### Electrons in Few-Layer Graphene: Evolution from a 2-Dimensional to a 3-Dimensional Material

**Kin Fai Mak**, *Columbia University, USA* | **Matthew Y. Sfeir**, *Brookhaven National Laboratory, Upton, USA* | **James A. Misewich**, *Brookhaven National Laboratory, Upton, USA* | **Tony F. Heinz**, *Columbia University, USA*

much recent theoretical study. Experimental investigations have, however, been limited primarily to single-layer graphene and a few studies in bilayer graphene. Here we identify Bernal-stacked FLG graphene crystals of layer thicknesses N = 1–8 and experimentally probe the band structure as it evolves, layer by layer, from the 2-dimensional (2-D) SLG towards the 3-dimensional (3-D) bulk solid. For each layer thickness N, infrared conductivity measurements reveal distinctive transitions which scale systematically with N. These observations can be explained within a unified zone-folding scheme that generates the electronic states for all FLG materials from that of bulk 3-D graphite crystal.

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### Charaterization of graphene grown on Ni

**Zonghai Hu**, *State key Lab for Artificial Microstructures and Mesoscopic Physics, School of Physics, Peking University* | **Xiuli Yin** | **Chenfang Lin** | **Nan Liu** | **Wen Ma** | **Jun Xie** | **Lei Fu** | **Zhongfan Liu**

Growth on metal surfaces is one of three major graphene making methods. The interactions between graphene and metal substrates greatly affect the electronic structure of graphene. This presentation focuses on characterization of monolayer and few-layer graphene grown on Ni surfaces either by segregation of carbon from metal bulk or gas phase decomposition of carbon sources (chemical vapor deposition, CVD). Various experimental techniques including low energy electron diffraction (LEED), Auger spectroscopy (AES), Raman spectroscopy, scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been used to study these samples. The results show effects of the coupling between graphene and Ni on the electronic structure of graphene.

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### Surfactant stabilised graphene dispersions at high concentration

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Graphene has generated intense research interest in recent years due to its unique physical properties. Our group has concentrated on producing liquid-phase dispersions of pristine graphene to facilitate materials processing and the development of graphene thin films. This submission focuses on the stable suspension of graphene at high concentration in aqueous media with the aid of the surfactant sodium cholate. This study compliments earlier work done by our team and others on surfactant-stabilised graphene. We show that under mild sonication for long times, graphene concentrations up to 0.3 mg/ml are attainable using just 0.1 mg/ml of surfactant. We studied the effect of centrifugation speed on the dispersions finding an empirical scaling of graphene concentration. We also used Raman spectroscopy and TEM analysis to assess the graphene quality and level of exfoliation. Finally, we show that high quality free-standing graphene films can be easily fabricated by our solution processing methods.

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### Propagative Landau states in carbon nanotubes

**Sebastien Nanot**, *Rice University, USA; LNCMI - Universite de Toulouse - France* | **Rémi Avriller**, *Universidad Autonoma de Madrid - Spain* | **Stephan Roche**, *CIN2 (CSIC-ICN) - Universitat Autonoma de Barcelona, Spain; CEA - Grenoble - France* | **Jean-Marc Broto**, *LNCMI - Universite de Toulouse - France* | **Bertrand Raquet**, *LNCMI - Universite de Toulouse - France*

We present evidence for the formation of unconventional, propagative Landau states in multiwalled carbon nanotubes in strong perpendicular magnetic fields up to 58 T. The existence of such propagative Landau states, as well as a reintroduction of backscattering in metallic tubes, was predicted by Ando and co-workers many years ago, and our experimental results confirm these predictions for the first time. Recent studies have unveiled the large energy dependence of the one-dimensional transport regime in individual carbon nanotubes (from ballistic to diffusive) through electrochemical potential tuning. In our study, we measured the conductance of individual multiwall nanotubes along with a control of the electrostatic doping in the back-gate field-effect transistor configuration. Our data demonstrate that an applied magnetic field drastically modifies the electronic band structure in agreement with theoretical calculations taking into account a homogeneous disorder. The conductance at high fields was found to converge to a gate-independent value for semiconducting shells, whereas for metallic shells all the curves were found to undergo significant conductance decay and converge toward a common quantum regime, irrespective of the electrostatic doping. We interpret this phenomenon in terms of energy gap closing in a semiconducting nanotube and the reintroduction of backscattering along with the pinning of the Fermi level to the zero energy Landau level in a metallic tube. These results reveal the onset of the first Landau state at zero energy (along with the density of state increasing) and the shift to higher energies of the dispersive subbands.

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### Understanding the origins of single walled carbon nanotube electron paramagnetic resonance

**Mujtaba Zaka**, *Department of Materials, QIPIRC, University Of Oxford* | **Jamie Warner**, *Department of Materials, QIPIRC, University Of Oxford* | **Arzhang Ardavan**, *Clarendon Laboratory, Department of Physics, QIPIRC, University Of Oxford* | **Mark Rümmeli**, *IFW Dresden, Germany* | **Andrew Briggs**, *Department of Materials, QIPIRC, University Of Oxford*

Current production methods produce SWNT with impurities such as amorphous and graphitic carbon and catalyst particles, thus inhibiting the true NT EPR to be determined. SWNT are used as an architect material for the filling of 1D ordered metallofullerenes forming peapod structures. EPR studies of the peapods system are limited due to the impurities of SWNT, and it is important that clean SWNT are prepared and their intrinsic EPR is understood. SWNTs produced by laser ablation are purified by microwave digestion and aqua-regia treatment or centrifugation and for arc discharge NTs high thermal annealing was employed. TEM, UV-Vis absorption, AFM, VSM compared the effects of the different purification methods, on the structural properties and the magnetic properties. Centrifugation of large diameter laser ablation SWNT successfully removed catalyst particles, and has further application in separating SWNT chiralities. The affects of catalyst particles and tube diameter are understood through comparative EPR of the raw and purified SWNT samples.  We have analysed each step in the purification process and compared the catalyst and impurity content with the EPR signal. We have elucidated that the EPR signal arises from catalyst particles and impurities rather than from high quality SWCNT.

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### Fingerprints of doped nanotubes : STM and quantum transport

**Luc Henrard**, *University Of Namur, Belgium* | **Bing Zheng**, *University Of Namur, Belgium* | **Hafid Khalfoun**, *University Of Namur, Belgium; Université Hassiba Benbouali, Chlef. Algeria* | **Patrick Hermet**, *University Of Namur, Belgium; University of Liege, Belgium* | **Sylvain Latil**, *CEA, France*

We report on studies of the electronic properties, STM and transport fingerprints of nitrogen and boron doped carbon nanosystems using density functional theory. The tunning of carbon nanotubes electronic properties are an important challenge for the design of nanoelectronic devices. The chemical doping is one of the possible methods to achieve such goal. Beside the physical properties of modified carbon materials, the knowledge of the experimental fingerprints of doping configuration is crucial to analyzed the experimentally produced samples. STM pattern and spectroscopy are obtained within a Tersoff-Hamann approach. Both nitrogen and boron substitutional doping, and more complex co-doping situation have been investigated. The doping type (n or p) and localized electronic states are determined and we show that the local patterns related to localized defects are similar for both planar graphene and tubular structures and do not strongly depends on the bias voltage. STM image obtained on the side of the tube opposite to the default is shown to be bias dependent. In an analysis of the quantum transport properties based on Landauer-Buttiker approach, we show that BN pairs are almost transparent for electron conductivity while B and N isolated defects reveal localization. A 'parity' effect (dependant on the relative number of B and N atoms in the defective structure) is demonstrate for larger domains. We also highlight that the reported transport properties obtained with ab-initio hamiltonian could be catched with a one-parameter model. This work is supported by the BNC-TUBE STREP EU project (Project Number 033350).

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### Electronic device fabrication with precisely placed carbon nanotubes of known chirality

**Christopher Allen**, *School of Physics and Astronomy, University Of Leeds, U.K.* | **Mark Elkin**, *School of Physics and Astronomy, University Of Leeds, U.K.***Can Zhang**, *Department of Electrical Engineering, Cambridge University, U.K.* | **Stephan Hofmann**, *Department of Electrical Engineering, Cambridge University, U.K.* | **Gavin Burnell**, *School of Physics and Astronomy, University Of Leeds, U.K.* | **John Robertson**, *Department of Electrical Engineering, Cambridge University, U.K.* | **Bryan Hickey**, *School of Physics and Astronomy, University Of Leeds, U.K.*

The electrical properties of single walled carbon nanotubes are strongly dependent on their precise atomic configuration and as such it is of great importance to be able to fabricate devices containing individual carbon nanotubes of known structure. We have developed a novel technique that allows for the determination of the chiral indices of an individual carbon nanotube followed by the precise placement of the tube onto pre-patterned electrodes. Carbon nanotubes are grown by chemical vapour deposition onto perforated TEM grids. Electron diffraction is performed on individual carbon nanotubes, the analysis of which reveals their structure. The desired carbon nanotube is then manipulated inside a combined STM-SEM system and placed with high precision onto pre-patterned electrodes. The electronic properties of the completed device are then studied in a field effect geometry both at room and cryogenic temperatures.

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### Performance Prediction of Graphene-Nanoribbon and Carbon Nanotube Transistors

**Michael Tan**, *Electrical Engineering Division and Centre for Advanced Electronics and Photonics, Engineering Dept., Cambridge University, UK* | **Gehan Amaratunga**, *Electrical Engineering Division and Centre for Advanced Electronics and Photonics, Engineering Dept., Cambridge University, UK*

Performance prediction of single wall carbon nanotube (SWCNT) and graphene nanoribbon (GNR) field-effect transistor (FET) performance is compared with each other, and to a 50nm channel length Si transistor. In particular the quasi one dimensional (Q1D) transport properties of the GNR-FET is compared to the SWNCT-FET. In both cases the possibility of ballistic transport allows the mitigation of short channel effects seen in Si transistors. The on-off ratio of the GNR-FET has improved to the point that transistor operation is warranted detailed analysis. By using a tight–binding energy dispersion approximation, the performance of semiconducting CNT and GNR is assessed in term of device specification, drain current drive strength, band gap and density of states. By reducing the maximum conductance 4e2/h by half, we observed that our model has particularly good fit with 50nm channel single walled carbon nanotube (SWCNT) experimental data. Given the same bandgap, SWCNT-FETs outperform GNR-FETs due to valley degeneracy. Nevertheless, the quality of device contacts will determine ultimate transistor performance, especially in terms of channel conductivity and hence output ON currents.

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### Electronic Structure of C59N-Enacapsulated Carbon Nanotubes

**Susumu Okada**, *University of Tsukuba*

We report total-energy electronic structure calculations that provide energetics of encapsulation of C59N azafullerene in the semiconducting carbon nanotube and electronic structures of the resulting carbon peapods. We find that the encapsulating process is exothermic for nanotubes of which diameter is larger than (17,0). We also find that the energy level of singly occupied state of azafullerene is strongly depends on the nanotube diameter. Furthermore, we clarify that the encapsulation of C59N molecules causes the substantial downward shift of the nearly free electron state of carbon nanotubes.

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### Conformational Analysis and Electronic Structure of Chiral Carbon and Carbon Nitride Nanotubes

**Ana Claudia Carvalho**, *GDENB - DFQ - ICE - Universidade Federal De Itajubá* | **Mariza Grassi**, *GDENB - DFQ - ICE - Universidade Federal De Itajubá* | **Cristiano Geraldo de Faria**, *DFQ - ICE - Universidade Federal de Juiz de Fora* | **Felipe Matuzalem**, *GDENB - DFQ - ICE - Universidade Federal De Itajubá*

Since their discovery in 1991, carbon nanotubes (CNT´s) have attracted several of experimental and theoretical studies. It is well known that the electronic structure of CNT´s could be further manipulated through a convenient doping process – the substitution of carbon atoms by other chemical species, such as nitrogen. These processes generate a new class of nanostructures with interesting electronic and mechanical properties: carbon nitride (CNx), CBy, and CxNyBz nanotubes.  Emission mechanisms, conduction, rectification and switching properties measured from carbon nanostructures are still under experimental and theoretical investigation. Relationship between morphology and electronic properties show controversial experimental results which difficult the development of new nanodevices based on nanometer-sized materials.  In this work geometry and electronic properties of chiral carbon and carbon nitride (CNx) nanotubes were investigated through semi-empirical and Density Functional Theory (DFT) methods. Carbon nitride (NTCNx) nanotubes were built through random substitution of carbon atoms by nitrogen in the network of carbon bonds. Our theoretical studies related to the replacement of carbon atoms by nitrogen atoms led us to conclude that the energy incorporation depends on the helicity of nanotubes. Density of States (DOS) results for pure carbon and NTCNx nanotubes, obtained through DFT and Hartree-Fock calculations, were analyzed. The introduction of nitrogen in the tube produce states in the gap region which characterizes the metallic behavior, as expected for these systems after N-doping. The authors would like to thank CENAPAD by the computational support and FAPEMIG for financial support.

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### Van der Waals Parameters for Small Diameter Carbon Nanotubes

**Markus Kaukonen**, *Aalto University*

Background The distance between individual nanotubes is important e.g. when considering electron tunneling between the tubes and when de-bundling of the bundles. It is determined by the van der Waals (vdW) interaction between the tubes. Design We have derived classical non-polarisable vdW force field parameters for small diameter (semi-)metallic and semiconducting carbon nanotubes. The fitting geometry consisted of two parallel nanotubes with wall--to--wall distances ranging from 2.6 to 8.5 Å. The fitting was done with respect to rigorous vdW--density functional theory (vdW-DFT) energies [1]. Similarly, the important carbon nanotube (CNT)--water parameters were fitted using single water molecule outside a single nanotube as the fitting configuration. Results The novel parameters were tested in a multitude of geometries including double-wall tubes, crossing tubes and nanotube--molecule interactions by comparison to full vdW-DFT calculation. The new force fields perform relatively well with neutral molecules but fail with charged molecules, double wall tubes and crossing tubes. Conclusion For the non-polarisable force fields the parameters for carbon nanotubes must be derived in very similar geometries compared to the application. On the other hand, it is found that the energy difference between the full vdW-DFT and the plain-DFT functionals is almost constant per carbon atom. This implies that the assumption of many force fields of rather universal vdW parameters may be justified. [1] Gulans, A.; Puska, M.; Nieminen, R. Physical Review B 2009, 79, 201105. Authors/Presenters M. Kaukonen, P. Havu, A. Gulans, E. Kauppinen

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### Energetics and Electronic Structures of Twisted Carbon Nanotubes

**Koichiro Kato**, *Tokyo Institute Of Technology*
**Takashi Koretsune**, *Tokyo Institute Of Technology* | **Susumu Saito**, *Tokyo Institute Of Technology*

Since the discovery of carbon nanotubes (CNTs), many experimental and theoretical works have been devoted to them. It is often thought CNT is a perfect cylinder made by rolling up a graphene sheet. In reality, however, there are undeniable possibilities that they possess structural deformations including twisted regions. As for chiral nanotubes, they may be twisted even at their ground state geometries because of their inherent helical structures. According to a density functional study, the electronic structures of CNTs sensitively depend on their geometry such as bond lengths and bond angles. Hence, electronic properties of deformed nanotubes should be of high interest and importance. In the present work, we study the energetics and electronic structures of twisted small-diameter single-walled CNTs in the framework of the density functional theory (DFT). In order to utilize the periodic boundary condition implemented in the conventional plane-wave DFT computational code, we study CNTs under several discretized twisting levels, and perform geometrical optimizations at each twisting level. In addition, we develop a real-space DFT computational code with helical-symmetry operation. We use it to optimize CNT geometries including twisting levels. We also report the twisting-level dependence of the electronic structures. Importantly, it is found that the fundamental gaps of some CNTs sensitively depend on twisting level.

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### Electrical Transport Properties of Carbon Nanotube filled with Fe Nanoparticles

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Carbon Nanotubes at low temperature behave as Quantum Dots for which charging processes become quantized, giving rise to Coulomb Blockade depending upon the coupling to the leads. Any small change in the electrostatic environment (tuned by the gate electrode) can induce shift of the stability diagram (so called Coulomb Diamonds) of the device, leading to conductivity variation of the Quantum Dot. A carbon nanotube can therefore be a very accurate electrometer1. For example, if a magnetic system is electronically coupled to a nanotube, its electron conduction may be influenced by the spin state of the magnetic system (magneto-Coulomb effect). Here we report on the electrical transport measurements of such hybrid systems where a carbon nanotube is filled with magnetic nanoparticles such as Iron (Fe). We find that low-temperature (~40mK) current-voltage measurements of such devices can show a hysteretic behaviour in conductance with sharp jumps at certain magnetic fields. We explain the results in terms of the magneto-Coulomb effect where the spin flip of the iron island at non-zero magnetic field causes an effective charge variation in the Nanotube due to the Zeeman energy. Our studies are a step forward towards the study of the magnetic anisotropy of individual nanoparticles. We believe our findings have important implications for sensitive magnetic detectors to study the magnetization reversal of individual magnetic nanoparticle or molecule, even weakly coupled to a carbon nanotube. Reference: 1. Bogani, L. & Wernsdorfer, W. Molecular spintronics using single-molecule magnets. Nat. Mater.7, 179-186 (2008).

## Poster Board | 111

### Surface induced enantiomeric selection in the adsorption of polycyclic aromatic hydrocarbons on Pt surfaces

**Giulio Biddau**, *Universidad Autonoma de Madrid* | **Gonzalo Otero**, *Instituto de Ciencia de Materiales de Madrid* | **Javier Mendez**, *Instituto de Ciencia de Materiales de Madrid* | **Jose Angel Martin-Gago**, *Instituto de Ciencia de Materiales de Madrid* | **Ruben Perez**, *Universidad Autonoma de Madrid*

Controlled synthesis of fullerenes and heterofullerenes on surfaces is a preceding step towards the development of a true fullerene-based molecular electronics. Here we analyze with surface-science techniques and first-principles methods the adsorption of the polycyclic hydrocarbons $C_{60}H_{30}$ and $C_{57}N_3H_{33}$ on Pt(111) surfaces. These PAHs have become particularly relevant after our recent publication showing that a catalysed cyclo-dehydrogenation process can transform these planar precursors with an almost 100% efficiency into $C_{60}$ fullerenes and triazafullerenes $C_{57}N_3$ [1]. Our study sheds light on the structure and interaction of these molecules upon adsorption on reactive substrates as Pt. In particular, we show that room-temperature deposition of these achiral molecules leads to surface induced chirality caused by the different landing side of the molecule, as depicted by in-situ scanning tunneling microscopy (STM) images that resolve the internal structure of the molecule. The surface becomes enantioselective “recognizing” the landing side of an individual molecule. Molecules adsorbed “right” or “left”-hand adopt two different orientations with respect to the surface crystallographic directions, shifted by about 35° between them. Large-scale DFT calculations reveal that this highly selective preferential orientation corresponds to a deep minimum in the potential energy surface for the configuration that maximizes the number of favorable adsorption positions for all of the individual carbon moieties. This mechanism operates in a particular molecule and therefore could be used to develop new routes for surface induced enantiomeric selection in cases where no crystalline domains with long-range order are formed. [1] G. Otero, et al, Nature 454, 865-869 (2008).

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### Processing and properties of aligned multi-walled carbon nanotube / aluminoborosilicate glass composites made by sol gel processing

**Geoffrey Otieno**, *University Of Oxford* | **Antal Koos** | **Frank Dillon** | **Richard Todd** | **Nicole Grobert**

We describe a novel sol-gel based approach for producing aluminoborosilicate glass composites containing continuous, aligned carbon nanotubes. The process involves the production of aligned carbon nanotubes (ACNT) via aerosol chemical vapour deposition (CVD), followed by infiltration of the ACNT with aluminoborosilicate sol. The advantages of this process are three fold: 1)aerosol CVD is an efficient method of producing clean, aligned arrays of CNTs, 2) sol-gel chemistry provides a simple route to infiltration of the ACNTs, and 3) carbon nanotube (CNT) agglomeration problems associated with CNT composites are circumvented. ACNTs (carpets) with heights of up to 4.4 mm were grown with areas of 10 mm x 20 mm for composite fabrication. The composite showed extensive pullout of the CNTs on a fracture surface and improved thermal and electrical conductivities of 16 Wm-1K-1 and 5~8 x 102 S m-1 respectively compared with only 1.2 W m-1 K-1 and 10-13 S m-1 for the monolithic glass.

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### Trifunctional Epoxy–SWCNT nanocomposite materials. The role of a block copolymer as a dispersing and reinforcing agent

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Nowadays, composite materials based on nanoreinforced polymers are at the forefront of the science and technology of high performance materials . The distribution of the reinforcing elements and their bonding to the polymer matrix are critical issues hindering the real potential of nano-reinforcements. In the present work, the preparation and characterization of nanocomposite materials based on an aerospace grade trifunctional epoxy and Single Walled Carbon Nanotubes (SWCNTs) is reported. The SWCNTs dispersion with an amphyphilic block copolymer (Pluronic F68) provided a highly disentangled reinforcer. The lyophilicity difference between the blocks allowed selectively controlling the miscibility of SWCNTs in the dispersion medium and in the epoxy resin. The dispersed SWCNTs exhibited a high miscibility in the epoxy resin which permitted the integration process to be carried out without solvents. The as-prepared nanocomposite materials showed a much more uniform dispersion of SWCNT within the epoxy matrix, as compared to those prepared without Pluronic F68. Pluronic-containing nanocomposites exhibited significant improvements in several properties including a toughness enhancement of 271%, an electrical conductivity increase of 7 orders of magnitude and a boosted thermo-oxidative stability. The results of this study demonstrate that the proposed method has been effective in improving mechanical, thermal and electrical properties of epoxy due to the enhanced quality of SWCNT dispersion.

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### Synthesis and characterization of polystyrene nanoparticles functionalized graphene/carbon nanotube hybrid composite

**Archana Patole**, *Department of Polymer Science and Engineering, Sungkyunkwan University* | **Shashikant P. Patole**, *SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University* | **Ji-Beom Yoo**, *SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University* | **Tae-Ho Kim**, *Department of Polymer Science and Engineering, Sungkyunkwan University*

This paper reports a large scale production route for polystyrene (PS) nanoparticles-functionalized graphene/carbon nanotubes (CNTs) hybrid composite using water based in situ microemulsion polymerization. The higher surface area of the graphene basal plane and the multiwall CNTs along with the better proximity of the reactant species in in situ microemulsion polymerization were used to functionalize the graphene and CNTs with PS nanoparticles. The electrical, thermal and mechanical properties of the composite films were studied. The modified graphene/CNTs complex exhibited good compatibility and interactions with the host PS matrix to form a new type of hybrid composite.

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### Transparent SWNT-PMMA Composites

**Robin Anderson**, *National Research Council Canada - Steacie Institute for Molecular Sciences* | **Karen Stoeffler**, *National Research Council Canada - Industrial Materials Institute* | **Behnam Ashrafi**, *National Research Council Canada - Institute for Aerospace Research* | **Vahid Mirjalili**, *Department of Mechanical Engineering, McGill University* | **Benoit Simard**, *National Research Council Canada - Steacie Institute for Molecular Sciences*

Single-walled carbon nanotubes (SWCNT) have significant promise as fillers for polymer reinforcement. To date, SWCNT have been incorporated into several polymers by various methods (melt mixing, solution processing, in situ polymerization, etc) with mixed results. The major hurdle that has to be overcome before the realization of the promise of SWCNT nanocomposites is dispersion in the matrix. PMMA based materials are useful in practically all segments of the economy, from household to automotive products, due to their toughness, stiffness, transparency and malleability. One drawback of PMMA materials for several applications is their weight. Incorporation of SWCNT into a PMMA matrix can result in a composite with increased toughness over the pure PMMA material. Less material can then be used to achieve the same properties. To obtain a well dispersed SWCNT-PMMA composite, we used a 2-step method which first functionalizes the SWCNTs with PMMA to produce a viscous “SWCNT-PMMA syrup”. This syrup is used as a starting material for either radical initiated polymerization of the monomer or to mix directly with commercially produced PMMA in solution. This method produces transparent, unaggregated composite materials with increased thermal stability over pure PMMA. Raman mapping and optical, transmission, and scanning electron microscopies clearly show the enhanced dispersion achieved by using the syrup. SWCNT-PMMA composites have also been characterized by TGA, DSC, and standard fracture and toughness tests.

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### Dispersion study of multi-wall carbon nanotubes synthesized by arc-discharge technique

**Marie Bourgeaux-Goget**, *n-Tec, Norway* | **Tomas-Roll Frømyr**, *Forsvarets forskningsinstitutt (FFI), Norway* | **Jean-Patrick Pinheiro**, *n-Tec, Norway* | **Finn Knut Hansen**, *Universitetet i Oslo, Norway*

Carbon nanotubes (CNTs) have received a great amount of interest because of their intrinsic and unique chemical, physical and mechanical properties that are suitable for versatile applications, especially for composite materials. Unfortunately, these materials are plagued with challenging dispersion protocols concomitant with difficult characterization techniques which complicate discovering their comprehensive properties in composite products. Our approach uses CNTs synthesized by arc-discharge technique as they offer fewer structural defects than those produced by other known techniques. A method was developed to characterize the dispersed medium using disc centrifuge for the detection of individual CNTs and residual aggregates. Studies performed on both pristine and purified CNTs show that interactions in between nanotubes are rather strong and high ultra-sound intensity is required to achieve complete dispersion of CNT bundles. Achieving such dispersion is a key advantage suggesting better properties on future composite materials.

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### Thermal and Electrical Conductivity of Composites with Covalent SWCNT-Epoxy Bonding

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Individual single-walled carbon nanotubes (SWCNTs) possess among the highest thermal and electrical conductivities of any material. The addition of CNTs to polymers routinely results in dramatic enhancements in electrical conductivity relative to the polymer matrix [1]. However, thermal conductivity is only slightly improved [2], and falls far short of early promise based on the filler geometry and properties. The small enhancements are attributed to a large interfacial thermal resistance associated with the CNT/polymer interface and covalent CNT-matrix bonding has been suggested as the most promising way to reduce this resistance [3]; however, covalent modification also decreases the electrical conductivity of the CNTs. Here we report preparation of SWCNT/epoxy composites with unmodified SWCNTs and with varying degrees of covalent bonding between the SWCNTs and the epoxy, achieved using the chemistry of reduced SWCNTs [4], along with thermal and electrical conductivity characterization of the resulting composites from room temperature to cryogenic temperatures. Thermal conductivity enhancements are limited by the low loading; however, the loading is sufficient to achieve electrical percolation. Thermal and electrical results are interpreted in terms of the effects of covalent bonding between the SWCNTs and epoxy, as well as literature models for CNT materials. [1] K.I. Winey et al. MRS Bull. 32(4), 348 (2007). [2] M.B. Jakubinek et al. Mater. Res. Soc. Symp. Proc. 1022, II03-06 (2007). [3] S.T. Huxtable et al. Nat. Mater. 2, 731-734 (2003); S. Shenogin et al. Appl. Phys. Lett. 85, 2229-2231 (2004). [4] Y. Martínez-Rubí et al. Chem. Commun. 5146-5148 (2007).

## Poster Board | 217

### Stochastic pore-blocking by ion transport through Single Walled Carbon Nanotube

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Biological signaling networks are able to utilize coherent and oscillatory signals from intrinsically noisy and stochastic components for ultrasensitive discrimination using stochastic resonance, a concept not yet demonstrated in man-made analogs. We show that the longest, highest aspect ratio, and smallest diameter synthetic nanopore examined to date, a 500 cm single walled carbon nanotube (SWNT), approximately 1.5 nm in diameter, demonstrates oscillations in electro-osmotic current at specific ranges of electric field, that are the signatures of stochastic resonance, yielding rhythmic and frequency locked signals. SWNT were grown on a SiO2 wafer and connected between two bonded, aqueous reservoirs at their plasma-etched and open ends. Stochastic pore blocking is observed when individual cations (Na+, Li+, K+, 1 M) partition into the nanotube during electro-osmosis, partially obstructing an otherwise stable proton current. We report the highest recorded proton conductivity experimentally observed (5x102 S/cm), suggesting an ordered water phase in the SWNT interior. The observed oscillations in the current occur due to a coupling between stochastic pore blocking and a diffusion limitation that develops at the pore mouth during proton transport. This is the first example of stochastic resonance in a synthetic nanopore, and illustrates how simple ionic transport can generate coherent waveforms within an inherently noisy environment, and points to new types of nano-reactors, sensors, and nanofluidic channels based on this platform.

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### Evaluation of Load Transfer Properties in Carbon Nanotube-Alumina Composites Using Single Fiber Pullout Experiments

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Carbon nanotubes (CNTs) are researched as reinforcing fillers in composites for their multifunctionality. The properties of such composites are dominated by the fiber bridging force resulting from debonding and sliding resistance, which dictates the major contribution to the strength and toughness. A fundamental understanding of the interface between a ceramic matrix and a filler component is of central importance for design of tougher ceramic composites. To date, the complete pullout of MWCNTs from ceramic composites has been postulated to occur with no breakage of the MWCNT, on the basis of SEM fracture surface observations. However, it was demonstrated from pullout experiments on a MWCNT-reinforced ceramic composite [1] using an in situ SEM method with a nanomanipulator system [2] that strong load transfer was revealed, and no pullout behavior was observed for all 15 MWCNTs. The MWCNTs broke in the outer-shells and the inner section was then pulled away, leaving the outer-shells of the companion fragment in the matrix. The measured fracture strengths of the MWCNTs ranged from 3 to 55 GPa (mean 17 GPa), quite similar to the tensile strengths of the MWCNT from the same sample used as filler in the composite (2 to 48 GPa; mean 20 GPa). Our finding suggests important implications for design of tougher ceramics with MWCNTs. The important factor for such tougher ceramics will thus be the use of gstrongh MWCNTs having higher mechanical performance. [1] G. Yamamoto et al., Nanotechnology 19, 315708 (2008). [2] M. F. Yu et al., Science 287, 637 (2000).

## Poster Board | 223

### Carbon nanotubes/Polyaniline Nanocomposites Studied by Resonant Raman Spectroscopy, FT-IR and Raman Spectroelectrochemistry

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The interest on the preparation of nanocomposites of carbon nanotubes (CNTs) and Polyaniline (PANI) has been tremendously increased in the last years due to the synergistic effects resulting from the combination of these two classes of materials. The nature of interaction between the CNT and PANI (a key-point to understand the properties of these materials) has been proposed in terms of $\pi$–$\pi$ interaction. This work reports the study of CNT/PANI nanocomposites by resonance Raman spectroscopy, FT-IR spectroscopy and Raman spectroelectrochemistry, aiming a fully understanding on the nature of the interaction between CNTs and PANI. Nanocomposites with different CNT/PANI ratio have been prepared through a novel interfacial polymerization route. This route yields self-assembled and transparent nanocomposite films. These films have been characterized by Raman spectroscopy using six excitation lines (441.6, 457.9, 488, 514.5, 568.2 and 647.1 nm), FT-IR spectra in attenuated total reflectance (ATR) mode, and Raman spectroelectrochemistry at different applied potential and two excitation lines (632.8 and 514.5 nm). The Raman spectra of nanocomposites show that the presence of CNTs stabilizes the more conductive polaronic structure of PANI. In all excitation lines, related changes were observed in the spectra. The same observations were also verified in the FTIR-ATR spectra, which show enhancement and red shift of polaronic modes, indicating more electronic delocalization. Results corroborate previous conclusions obtained by other techniques indicating a strong interaction between the components, characterized by a n-doping of CNTs by the PANI. ACKNOWLEDGMENTS: Brazilian Network on Carbon Nanotube Research, INCT-Nanocarbon, CNPq, CAPES/PROCAD.

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### Polypyrrole - Nanotube Composites

**Thea I. W. Reumann**, *Technical University Hamburg-Harburg* | **Karl Schulte**, *Technical University Hamburg-Harburg* | **Krzysztof K. K. Koziol**, *Department of Materials Science and Metallurgy, University of Cambridge, UK* | **Alan H. Windle**, *Department of Materials Science and Metallurgy, University of Cambridge, UK* | **Tim Burstein**, *Department of Materials Science and Metallurgy, University of Cambridge, UK* | **Graeme Smith**, *Department of Materials Science and Metallurgy, University of Cambridge, UK*

This work focuses on the electrochemical coating of multiwalled carbon nanotubes (MWCNT) arrays with Polypyrrole (PPy). The advantages of aligned arrays MWCNT over randomly orientated MWCNTs is already described for many applications. For this application especially the extreme high surface of the MWCNT array is very useful for depositing a thin PPy film, that still provides an open, porous structure. PPy as an electrically conducting polymer has been intensively studied over the last 30 years. The performance of conducting polymers is limited by the kinetics of the charging-discharging process (ion migration) hence the thickness and morphology of the polymer film plays an important role. The synthesis of the PPy-MWCNT Composites follows the electrochemical route. The MWCNT arrays were synthesized on a silicon wafer covered with a native oxid layer, which became during the coating process the working electrode. Potentiostatic and –dynamic experiments were performed in aqueous KCl solutions. The CNT-PPy film thickness and morphology was analyzed using scanning electron microscopy (SEM). Cyclic voltammetry (CV) studies were used to estimate the speed of the redox process and electrical impedance spectroscopy (EIS) for measuring the electrical resistance.

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### Single-walled Carbon Nanotubes as a Molecular Container in Gel and their Controlled Releasing Triggered by Near-IR Irradiation

**Tsuyohiko Fujigaya**, *Kyushu Univ.* | **Tatsuro Morimoto**, *Kyushu Univ.* | **Naotoshi Nakashima**

We prepared a series of single-walled carbon nanotubes (SWNTs)-embedded composite gels by the gelation of acrylamide derivatives in the presence of the SWNTs dispersed in sodium dodecyl benzenesulfonic acid sodium salt (SDBS) aqueous solution. We found the SWNTs remained isolated even after the removal of SDBS in poly(N-isopropylacrylamide) (PNIPAM) gel, while SWNTs in polyacrylamide (PAA) gel ended up with the small bundling of the SWNTs. Exposed SWNT surface in PNIPAM gel thus obtained was utilized as a scaffold for adsorption of small molecule, doxorubicin hydrochloride (DOX). From the comparison between the SWNT/PNIPAM composite gel and PNIPAM gel, it is revealed that SWNT surfaces in the composite gel served as a molecular container to held DOX molecules effectively in basic aqueous media. By lowering the pH of the aqueous media, DOX molecules held on SWNT surface were efficiently released to outside of the gel. In addition, we realized the light-induced quick releasing of the DOX from the composite gel owing to the photothermal conversion effect of the SWNTs.

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### Alternative Route for the Synthesis of Selenium-Carbon Nanocables

**Eduardo Barros**, *Universidade Federal Do Ceará* | **Gilberto D. Saraiva**, *Universidade Federal Do Ceará; Universidade Estadual do Ceará* | **Oscar E. D. Rodrigues**, *Universidade Federal de Santa Maria* | **Rafaella O. Nascimento**, *Universidade Estadual de Campinas* | **A. L. Braga**, *Universidade Federal de Santa Catarina* | **Yoong Ahm Kim**, *Shinshu University* | **Morinobu Endo**, *Shinshu University* | **Antonio G. Souza Filho**, *Universidade Federal Do Ceará*

Chemical manipulation of single wall carbon nanotubes (SWNTs), especially sidewall functionalization, has recently become an area of fundamental interest. Additionally, Selenium exhibits a unique combination of many interesting and useful properties, such as a high photoconductivity, nonlinear optical response and a high flexibility to react with a number of chemicals affording a series of very functional selenides such as ZnSe and CdSe. In this context, the preparation of a new hybrid system employing one-dimensional selenium nanostructures and carbon nanotubes allow for a very interesting system for technological applications. In a previous publication, [1] we have prepared a new selenium-carbon nanocable employing a carbanionic intermediate species which afforded a covalent interaction between the SWNT and the Se-nanowires (Se-NW). To explore the possible routes for promoting the interaction between selenium and carbon nanotubes in order to form hybrid nanomaterials we combine here a new synthesis strategy, allowing a Se-NW growth by using HipCo Carbon nanotubes for physical support. The resulting material was characterized by Raman spectroscopy and Transmission electron microscopy and was found to be composed of carbon nanotube bundles wrapped up by thin helical selenium nanowires. [1] O.E.D. Rodrigues et al. Nano Lett. 8, 3651 (2008).

## Poster Board | 235

### Development of CNT/photopolymer nanocomposites and evaluation of dispersion state of CNT on thermal conductivity of the nanocomposites

**Tsuyohiko Fujigaya**, *Kyushu Univ.* | **Takahiro Fukumaru**, *Kyushu Univ.* | **Naotoshi Nakashima**, *Kyushu Univ.; JST-CREST*

Carbon nanotubes (CNTs) have attracted attention because of their excellent electronic, thermal and superior mechanical properties. Great efforts have been made on CNT/polymer composites to incorporate CNTsf properties with host materials. However, CNTs are difficult to disperse to polymer matrix for practical applications because of their rigidly and strong van der Walls interaction between CNTs. In this poster, We describe i) the evaluation of bundled degrees of single-walled carbon nanotubes (SWNTs) in SWNT/UV-curable resin composite films based on the intensity change in the radial breading mode (RBM) of their Raman spectra at a 785-nm excitation, and ii) the thermal conductivity measurements of the composite films using the temperature wave analysis method. The homogeneous dispersion of the SWNTs produced a gradual increase in the thermal conductivity with an increase in the SWNT loading up to 5.0 wt%. This observed behavior is quite different from that of the electric conductivity of the composite films, in which the electric conductivities dramatically decrease at around only a 0.05 wt%-SWNT loading.

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### Ostwald Ripening of Iron (Fe) Catalyst Nanoparticules on Aluminum Oxide Surfaces (Al2O3) for the Growth of Carbon Nanotubes

**Roberto Acosta**, *Air Force Research Laboratory* | **Gordon Sargent**, *Air Force Research Laboratory* | **Lee Semiatin**, *Air Force Research Laboratory* | **Benji Maruyama**, *Air Force Research Laboratory*

Theoretical models have proposed that the nucleation and growth mechanism of carbon nanotubes (CNTs) has been affected by the catalytic activity of transition metals. The catalyst behavior during growth has been mainly associated as the responsible mechanism for the termination of CNT growth. Although several hypotheses have been developed to explain this mechanism, is still today an unresolved phenomenon. The Ostwald ripening mechanism was further investigated as a function of thermal annealing in Hydrogen (H2) for iron (Fe) catalyst nanoparticles on various surfaces of aluminum oxide. Experimental results showed that the growth kinetics of Fe nanoparticles on aluminum oxide obeyed the Ostwald ripening mechanism. The proportionality constant (K) for the kinetic equation of the Lyfshitz-Slyozov-Wagner (LSW) theory was calculated for sputtered alumina and sapphire. The log-normal particle size distribution for the Fe nanoparticles was studied as a function of annealing time in H2 for 5, 10, and 15 minutes. Then, after the growth of SWNTs, the particle size distribution of Fe was also investigated on C- and A- face sapphire surfaces. The synthesis of SWNTs resulted in randomly oriented tubes on the C- face sapphire; as opposed to aligned tubes on the A- face sapphire surfaces. The SWNTs aligned along the specific crystalline directions corresponding to the anisotropic pseudo-1D array of Al atoms on the sapphire surface. The Ostwald ripening effect and the synthesis of SWNTs, was characterized by atomic force microscopy (AFM), scanning electron microscopy (SEM), and Raman Spectroscopy.

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### Formation of aligned carbon nanotube monolayer films by the Langmuir-Blodgett technique

**Azin Fahimi**, *University Of Surrey* | **Chiara Bo**, *University Of Surrey* | **Izabela Jurewicz**, *University Of Surrey* | **David Faux**, *University Of Surrey* | **Alan Dalton**, *University Of Surrey*

Carbon nanotubes (CNTs) are materials with a variety of fascinating properties related to their interesting quasi-one-dimensional electronic structure. There is considerable interest in developing economical and practical methods for producing aligned CNTs and utilizing them in electronic components, optical waveguides and optoelectronic devices. More recently, CNTs have inspired a great deal of interest as potential candidates for transparent electrodes in solar cells due to their high conductivity. The Langmuir-Blodgett (L-B) technique has proved effective in producing monolayers of carbon nanotubes [1]. Based on L-B assembly, we describe a method to control the alignment and connectivity of CNTs in large-area films. Dispersions of SWNTs as a function of concentration were prepared by dispersing in chloroform solutions of a conjugated polymer, poly (mphenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) (PmPV), which has been used extensively for optoelectornic applications. Moreover, we have previously shown that PmPV is an excellent dispersant for CNTs [2]. The L-B technique was used to deposit monolayers of aligned polymer wrapped SWNTs onto a substrate. The alignment was controlled by varying experimental parameters including spreading volume, compression speed and the number of deposition cycles. Microscopy (SEM, AFM) as well as polarized Raman spectroscopy investigations showed that the CNTs alignment can be improved if surface pressure during deposition is increased and the optimum number of compression-expansion hysteresis cycles prior to depositing is performed. The electrical conductivity and photoconductivity of the resulting monolayer were investigated and compared to existing technologies. Applications are discussed. 1 Xiaolin Li, JACS,2007 2 Dalton A.B, Journal of Photochemistry and Photobiology a-Chemistry,2001

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### Prevention of Photoreduction in Confined Nanospace of Carbon Nanotubes

**Keita Kobayashi**, *National Institute Of Advanced Industrial Science And Technology* | **Kazu Suenaga**, *National Institute Of Advanced Industrial Science And Technology* | **Takeshi Saito**, *National Institute Of Advanced Industrial Science And Technology; PREST, Japan Science and Technology* | **Hisanori Shinohara**, *Department of Chemistry & Institute for Advanced Research, Nagoya University* | **Sumio Iijima**, *National Institute Of Advanced Industrial Science And Technology*

The stable pseudo-one-dimensional confined nanospace of carbon nanotubes (CNTs) can serve as an ideal environment for template assembly of various nano-materials [1, 2]. Since the confined nanospace of CNTs prevents molecules from reacting, as it impedes their movement, it can potentially be utilized for stable storage of various reactive materials [3, 4]. In this study, we report that the silver bromide (AgBr) nanowires within single-wall carbon nanotubes (SWCNTs) are extremely stable under the UV laser light illumination in comparison with the photosensitive AgBr bulk powder. The confined structure of AgBr nanowires within SWCNTs (AgBr@SWCNTs) confirmed by high resolution transmission electron microscopy (HRTEM) does not allow the photoreduction to the silver (Ag) by preventing the migration of bromine (Br) and silver (Ag) atoms. The reduction of AgBr nanowires to the Ag can be observed only when the outer SWCNT has a large defective area. An in situ HRTEM and EDX study of such a photoreaction suggests that the Br atoms indeed migrate through the defect of SWCNTs.  References [1] P. M. Ajayan and S. Iijima, Nature, 361, 333 (1993). [2] J. Sloan et al., Chem. Commun., 1319 (2002). [3] D. Nishide et al., Chem. Phys. Lett., 428, 356 (2006). [4] Z. Liu et al., Nat. Mater., 2, 422 (2007). e-mail: kobayashi-z@aist.go.jp

## Poster Board | 246

### Magnetic force microscopy studies of Fe- and Fe3C-filled MWNT

**Matthias Lutz**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Uhland Weissker**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Franziska Wolny**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Markus Löffler**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Thomas Mühl**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Silke Hampel**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Albrecht Leonhardt**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Bernd Büchner**, *Leibniz Institute for Solid State and Materials Research IFW Dresden* | **Rüdiger Klingeler**, *Leibniz Institute for Solid State and Materials Research IFW Dresden*

We present studies on the magnetic properties of Fe- and Fe3C- filled Multi-Wall Carbon Nanotubes (MWNT) synthesized by Chemical Vapour Deposition (CVD). Magnetic Force Microscopy (MFM) as well as Transmission and Scanning Electron Microscopy (TEM & SEM) are employed to study the magnetic and structural properties of these single domain magnetic nanowires encapsulated by MWNT. The cylindrical form imposed by the CNT is responsible for a high shape anisotropy, dominating the magnetic properties of the Fe nanowires, leading to switching fields between 100-400 mT. Fe3C features a strong magneto crystalline anisotropy, which dominates over the shape anisotropy. The Fe3C nanowires crystallize in a controlled way because the rigid and temperature stable CNT acts as a mould, it only allows expansion along the hollow of the tube. The magnetic easy c-axis forms perpendicular to the long wire axis, leading to a transverse magnetization with switching fields of the order of 40 mT. Filling MWNT utilizes some of their main advantages: the carbon shells offer mechanical protection as well as chemically isolating the filling and the environment. In addition it is possible to chemically and biologically functionalize the exterior carbon shells without affecting the filling. Their chemical stability is also responsible for long term stability of the filling's magnetic properties by preventing oxidation as well as averting a potential toxicity of the filling in a biological setting. These properties make magnetically functionalized MWNT excellent candidates for applications such as: data storage, MFM tips and hyperthermia agents for targeted cancer treatment.

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### Experimental study on chirality changes of isolated carbon nanotubes in superplastic deformation process

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Superplasticity of single wall carbon nanotubes (SWCNTs) has been reported by Huang et al.; SWCNTs are elongated much than 200%

by applying tensile stress as well as slight amount of current [1]. Such a deformation has been theoretically discussed on the basis of the dislocation theory; topological defects consisting of a pair of 5- and 7-membered rings (5-7 defect) are migrated by switching carbon-carbon bonds in the SWCNT, so that the chiral index is changed [2]. In the present study, we experimentally investigated the changes in chiral indices of nanotubes during the superplastic elongation process by means of nanobeam electron diffraction [3]. In a transmission electron microscope with 90 kV acceleration voltage, isolated nanotubes were bridged between a specimen stage and a tungsten probe. The nanotube were then pulled by operating the tungsten probe with applying current by approximately 1 μA/nm. As the result, we successfully observed the elementary step of structural change in plastic deformation process, which correspond to the migration of a couple of 5-7 defect. In addition, we found that the all layers constituting a multi-wall carbon nanotube are simultaneously elongated. The experimental result of chirality analysis suggested existence of interlayer correlation in the changes of chiralities. [1] J. Y. Huang, et al., Nature 439: 281 (2006). [2] B. I. Yakobson, Appl. Phys. Lett., 72: 918 (1998). [3] K. Hirahara et al., submitted.

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### Aggregation dependent Photoluminescence Sidebands in Single Walled Carbon Nanotube

**Yuan Chen**, *Nanyang Technological University* | **Li Wei**, *Nanyang Technological University*

Aggregation of single-walled carbon nanotubes (SWCNTs) is one of the major obstacles for many nanotube fundamental studies and practical applications, such as nanocomposites, electronic devices, bioimaging, biosensors and drug-delivery. In this study, we showed that photoluminescence (PL) sidebands (the transverse sideband E12,21, the phonon coupled sidebands E22+G,G' and the E33-E11 emission band) are dependent on the aggregation of single-walled carbon nanotubes (SWCNTs). Two SWCNT samples enriched with (6,5) and (7,5) chiral structures were employed to establish the correlation between PL sidebands and nanotube aggregation. SWCNT suspensions containing various fractions of bundles were obtained by ultracentrifugation. Dialysis was used to achieve the controlled nanotube re-bundling. We interpret the observed PL sideband changes are because of the aggregation-dependent changes in their exciton relaxation routes. Furthermore, the aggregation¨Cdependent PL sidebands were also demonstrated in diverse dispersion conditions involving different surfactants and solvents. The results highlight the potential of employing PL sidebands as sensitive characterizing tools for monitoring the nanotube aggregation under different circumstances.

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### Theoretical studies of topological defects in carbon nanostructures

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The formation energies of topological defects such as single Stone-Wales, single mono-vacancy and single di-vacancy defects in single and double layers graphite has been investigated using B3LYP and B2PLYP functional. The formation energies were computed and the full analysis of the transition state for each defect were done. The transition state of the generated Stone-Wales defect in the graphene with approximately 100 carbon atoms were analysed. In the case of the mono- and di-vacancy defects, their transition states for the double layers carbon structures with approximately 200 atoms were analysed, as well. In addition, the optimisation of these flat carbon structures and the curved fragment of (17,13) single-walled carbon nanotubes (more than 400 atoms) containing three types of topological defects were performed by combining the classical molecular dynamic simulations using the REBO2 (the reactive bond order potential) potential with the density functional theory using B3LYP functional and the MP2 methods. Finally, the HOMO-LUMO molecular orbitals calculated using the 6-311g* basis set for such planar and curved defected carbon nanostructures were compared.

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### Microphotoluminescence of hexagonal boron-nitride crystals and boron-nitride nanotubes

**Aurélie Pierret**, *ONERA - The French Aerospace Lab (Department LEM)* | **Gurvan Brasse**, *ONERA - The French Aerospace Lab (Department LEM)* | **Sylvain Maine**, *ONERA - The French Aerospace Lab (Department LEM)* | **Brigitte Attal-Tretout**, *ONERA - The french Aerospace Lab (Department DMPH)* | **François Ducastelle**, *ONERA - The French Aerospace Lab (Department LEM)* | **Annick Loiseau**, *ONERA - The French Aerospace Lab (Department LEM)*

Hexagonal Boron-Nitride (hBN) and BN nanotubes (BNNTs) present a large potential for optical applications in the UV range since they have a wide bang gap (>=5.8 eV). Their emission is governed by excitonic effects between 200 nm and 250 nm and by impurities around 300 nm as shown by previous theoretical and experimental studies. Because of the paucity of BN materials, very few studies exist on their optoelectronic properties, which are not yet well understood. Given the similarities between hBN and multi-wall BNNTs with a high number of walls, the critical point is the observation of BNNTs with a reduced number of walls (less than ten) in order to confirm theoretical predictions concerning the confinement effects due to their reduced sizes. The studies of such wide band gap semiconductor materials requires specific experimental equipments suited to the UV range, while a higher attention is paid to observe single-wall BNNTs. By this way, a microphotoluminescence experimental setup has been developed by using an excitation at 193 nm. Thanks to a higher spatial resolution and improved signal-to-noise ratio on the detection channel, we are now able to detect low luminescent objects in the UV range, as BNNTs with a few number of walls and recent advances are related in this communication.

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### Mechanical Properties of iron-filled Carbon Nanotubes

**Uhland Weissker**, *Leibniz Institute for Solid State and Materials Research, Germany* | **Markus Löffler**, *Leibniz Institute for Solid State and Materials Research, Germany* | **Franziska Wolny**, *Leibniz Institute for Solid State and Materials Research, Germany* | **Thomas Mühl**, *Leibniz Institute for Solid State and Materials Research, Germany* | **Albrecht Leonhardt**, *Leibniz Institute for Solid State and Materials Research, Germany* | **Bernd Büchner**, *Leibniz Institute for Solid State and Materials Research, Germany*

Iron-filled carbon nanotubes (Fe-CNT) represent a class of promising nanoscale materials with extraordinary mechanical and magnetic properties. It was shown that the carbon shells protect the encapsulated nanowires from oxidation and ensure a high mechanical stability. In this study mechanical properties of single Fe-CNT were analysed by dynamic and static bending methods. In the first method the Young's modulus was determined by evaluating the eigenfrequency and the envelope curve of the resonant vibrating state. The static bending experiments were performed inside a transmission electron microscope (TEM) employing a scanning probe microscopy holder (Nanofactory). The developed simple setup allowed the measurement of the stiffness of a single CNT. Single CNTs were pressed against a soft conventional atomic force cantilever. The force as well as the bending curve of the CNTs was obtained from TEM micrographs. For both methods the CNT mounting on the sample holder had to be carefully considered. In this study it was modelled as a torsion spring and included in the calculation of the effective Young's modulus. The Young's moduli of iron filled carbon nanotubes are comparable to those of unfilled multi-walled carbon nanotubes with similar outer diameters and shell structures.

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### Photoluminescence and Raman Spectroscopy On CVD Grown Single-Walled Carbon Nanotubes: Strain And Relaxation Effects

**Ninette Stürzl**, *Karlsruhe Institute Of Technology*

Horizontally aligned, individual single-walled carbon nanotubes (SWNTs) were grown on Si/SiO2 substrates by applying chemical vapor deposition (CVD) at very low feeding gas flow rates at 970°C [1] and characterized by scanning electron (SEM), atomic force (AFM), Raman and photoluminescence (PL) microscopy [2]. In particular, strain effects on SWNTs were investigated in this work by means of Raman and PL microscopy. Strain in SWNTs results initially from an interplay between thermal compression of a tube and a substrate (by cooling down from the process to room temperature) as well as their interactions (adhesion of the tube to the substrate). Strain was also induced and relaxed in selected nanotube sites by their mechanical manipulation (bending, rupture) with an AFM tip. Furthermore, a focused ion beam (FIB) was applied as a well-defined cutting tool for SWNTs. Strain relaxation was observed for the FIB-cut ends of nanotubes. [1] Z. Jin et al., Nano Lett. 7, 2073 (2007) [2] O. Kiowski et al., Phys. Rev. B, 80, 075426 (2009)

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### Dramatically improved load-bearing capability of multi-walled carbon nanotubes in the ceramic environment

**Mehdi Estili**, *Tohoku University* | **Akira Kawasaki**, *Tohoku University*

Multi-walled carbon nanotube (MWCNT) with exceptional load-bearing capability and large aspect ratio is an alternative reinforcement to improve mechanical response of conventional ceramics. However, high temperatures and pressures involved in techniques for the incorporation of MWCNT into the ceramic environment and that compressive stress applied from the ceramic matrix may effectively change the original mechanical response of MWCNT when embedded in ceramic-based materials. We studied load-bearing capability of MWCNTs in the ceramic environment in tensile/bending modes employing piezoelectric nano-positioners equipped with cantilever-based force sensors. We have realized a dramatic improvement in load-bearing capability of MWCNTs, which can be explained by the reversible in-wall irregularities engineered in MWCNT structure by the compressive stress applied from the ceramic matrix. These irregularities cause strong inter-wall shear resistance leading to reduction of load on the outermost wall and distribution among the inner walls. Our results show that MWCNTs retain their improved load-bearing capability even in highly deflected configurations in the ceramic environment. Our findings suggest that the strength of MWCNTs increases dramatically in the ceramic environment, i.e., that MWCNTs are strongly effective to reinforce ceramic-based materials.

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### Raman probing of uniaxial strain in individual single-wall carbon nanotubes in a composite material

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The temperature dependence of the Raman spectrum of a gelatine-based composite material doped with single-walled carbon nanotubes is reported. A significant up-shift of the G-mode frequency is observed when the temperature is decreased from room temperature to 20 K. This frequency shift is significantly stronger than the one found for pure thermal effects. In contrast, the radial breathing modes display no significant shift in the same temperature range. These results are well understood by considering a uniaxial strain on the nanotube induced by the thermal expansivity mismatch between the nanotube and the surrounding matrix.

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### Characterisation of carbon nanotube solutions by image analysis

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Precise quality control systems of industrial process require real-time characterisation techniques that allow the establishment of in-line statistical process control (SPC). Due to its simplicity, digital image processing is a particularly attractive technique. In this work we report on the characterisation of solutions of carbon nanotubes in N-methyl-2-pyrrolidone (NMP) by image analysis. It has been previously reported that the degree of dispersion of CNTs (and graphene) in amide solvents depend on the free energy of mixing, which in turn, depend on the total CNT-solvent surface energies. However, for solvents with sufficiently strong interaction energies with CNTs, a high local ordering does not occur at the interface, and thus the free energy of mixing will depend almost exclusively on the enthalpic contribution. As a consequence, an equilibrium concentration of dispersed CNTs will not necessarily follow the nominal concentration of the solution. Single-walled CNT-NMP solutions of various nominal concentrations were prepared by a standard procedure including sonication, centrifugation and filtering. Digital images were taken with identical lighting conditions. The analysis procedure was: (i) selection of uniform portion based on grey values limits; (ii) Background light subtraction based on low-pass kernel; (iii) Gaussian blur the output value is the distribution peak. Our initial results show that the minimum output grey value for a given concentration series does not occur for the minimum nominal concentration. This suggests that it is possible to correlate the output grey value to the free energy of mixing CNTs and solvents, therefore calculate the real concentration achieved.

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### Spectroscopic Characterization of Bile Salt Solubilized Single-Wall Carbon Nanotubes and Nanohybrids

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Bile salts (e.g. [tauro/deoxy]cholate) are amazing surfactants for the solubilization of SWCNTs in water,[1] yielding much higher concentrations of individual SWCNTs, and forming homogeneous coatings around the SWCNTs resulting in unusually high resolution in optical spectroscopy. The high resolution in 2D Raman maps allowed us to resolve empty (end-capped) and water-filled (opened) SWCNTs[2], which we used to demonstrate single-file water filling of SWCNTs for the first time, down to extremely thin (5,3) tubes. Bile salt solubilization is also very useful in the preparation of purified nanohybrids of SWCNTs coated with Co(II) porphyrins[3], and in the preparation of stretch-aligned SWCNT/polymer composites, which we applied in the EPR spectroscopic characterization of SWCNTs filled with Cu(acac)2 complexes[4], yielding information on the orientation, spacing, and environment of the encapsulated complexes. [1] W. Wenseleers, I.I. Vlasov, E. Goovaerts, E.D. Obraztsova, A.S. Lobach, A. Bouwen, 'Efficient isolation and solubilization of pristine single-walled nanotubes in bile salt micelles' Adv. Funct. Mater. 14, 1105-1112 (2004). [2] W. Wenseleers, S. Cambré, J. Culin, A. Bouwen, E. Goovaerts, 'Effect of water filling on the electronic and vibrational resonances of carbon nanotubes: Characterizing tube opening by Raman spectroscopy' Adv. Mater. 19, 2274-2278 (2007). [3] S. Cambré, W. Wenseleers, J. Culin, S. Van Doorslaer, A. Fonseca, J.B.Nagy, E. Goovaerts, 'Characterisation of nanohybrids of porphyrins with metallic and semiconducting carbon nanotubes by EPR and optical spectroscopy' ChemPhysChem 9, 1930-1941 (2008). [4] S. Cambré, W. Wenseleers, E. Goovaerts, 'Endohedral Copper(II) acetylacetonate/Single-Walled Carbon Nanotube Hybrids Characterized by Electron Paramagnetic Resonance' J. Phys. Chem. C 113, 13505-13514 (2009).

## Poster Board | 258

### General Equation for the Determination of Defect Density in Monolayer Graphene by Raman Spectroscopy

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The one-phonon Raman spectrum of graphene shows a single peak centered at 1580 cm-1, called G band. However, the presence of structural disorder that breaks the translational symmetry gives rise to an additional feature centered at 1350 cm-1 (for excitation laser energy of 2.41eV), usually called D band. In this work we have performed a systematic Raman study of distinct monolayer graphene samples which have been exposed to different doses of ion-bombardment. We have measured the average distance L_D between two point defects created from the impact of the ions on the graphene lattice. For that, we have used scanning tunneling microscopy (STM). By comparing the STM data with the Raman spectrum of each respective sample using different incident laser energies, we have observed that the ratio between the D and G bands intensities (ID/IG) multiplied by the fourth power of the incident laser energy E_L is inversely proportional to L_D^2 for samples with L_D > 5 nm. Based on the experimental results we have generated a general equation to measure the average distance L_D between two point defects in monolayer graphene using the I_D/I_G for any excitation laser energy E_L in the visible range.

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### The effect of barrier layer-mediated catalytic deactivation in vertically aligned carbon nanotube growth

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The dependence of the growth kinetics of carbon nanotubes (CNTs) on the size of the Fe-catalyst in the H2 assisted atmospheric pressure chemical vapor deposition was studied. A growth interruption method was used to determine the in situ growth rate. The formation of a compact scale contaminant layer around the catalyst hinders the diffusion of the reactant species required to grow the CNTs. The high temperature metal oxidation behavior observed using parabolic curve fitting was attributed to the size dependent catalyst activity. The parabolic rate constant shows linear dependence on the catalyst size. Details of the analysis are presented.

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### Growth of CNTs carpets on substrates with different oxide interlayers – a comparative study

**Vyacheslav Khavrus**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Albrecht Leonhardt**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Joachim Schumann**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Rainer Kaltofen**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Steffen Oswald**, *Leibniz Institute For Solid State And Materials Research Dresden*

Carbon nanotubes (CNTs) have been recognized as a novel material with many potential applications in chemical technology, sensors, and nanoscale electronics. Vertically aligned CNTs grown on conductive substrates are of great interest for development novel application like supercapacitors, flat panel displays and interconnects requiring good electrical contact to the nanotube. Direct growth of CNTs on metal substrates is a great challenge due to formation of inactive alloys with catalyst nanoparticles (usually Fe, Co, or Ni) and microstructural changes of metal surface above the Tammann temperature that disallows formation of catalyst nanoclusters needed for nanotube growth. SiO2 and Al2O3 are commonly used interlayers for promoting growth of aligned CNTs on different substrates. However, such interlayers have a low electrical conductivity which limits application of prepared composites. It was found recently that Cr2O3, an electrically conductive oxide, can be also a promoter for growth aligned CNTs, however, their length is shorter in comparison to SiO2 or Al2O3 [1,2]. In our work, we have compared growth of CNTs on substrates with different oxide interlayers (SiO2, Al2O3, Cr2O3) with sputtered Fe particles by the CVD of ethylene. Optimal conditions of CNT formation in dependence on parameters of oxide interlayers were determined. Properties of synthesized materials were characterized by scanning and transmission electron microscopy, X-ray photoelectron and Raman spectroscopy. The mechanism of each interlayer action on the morphology of CNT carpets is discussed. [1] S. K. Pal et al. Carbon 48 (2010) 844–853. [2] X. Cui et al. Carbon 47 (2009) 3441–3451.

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### The Mechanism of Single-Walled Carbon Nanotube Growth and Chirality Selection Induced by Carbon Atom and Dimer Addition

**Yuan Chen**, *Nanyang Technological University* | **Qiang Wang**, *Nanyang Technological University* | **Shuo-Wang Yang**, *Institute of High Performance Computing, Singapore*

Based on abounding density function calculations, a mechanism is proposed to explain single-walled carbon nanotube (SWCNT) growth and chirality selection induced by single C atom and C2 dimer addition under catalyst-free conditions. Two competitive reaction paths, chirality change induced by single C atom and nanotube growth through C2 dimer addition, are identified. The structures of the intermediates and transition states along the potential energy surfaces during the formation of near-armchair (6,5), (7,5), (8,5) and (9,5) caps initiated from the armchair carbon cap (5,5) are elucidated in detail. The results show that the direct adsorptions of C atom or C2 dimer on growing carbon caps show no energy barrier. Moreover, the incorporations of adsorbed C atom or C2 dimer display low energy barriers, indicating SWCNT growth and chirality change are thermodynamically and kinetically feasible under catalyst-free growth conditions. In addition, the results also highlight that the concentrations of C atoms and C2 dimers in the experimental environment would play a critical role in the chiral-selective SWCNT synthesis. Potential opportunities exist in achieving the (n,m) selective growth by delivering single C atom or C2 dimers at different ratios during different reaction stages.

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### Low Temperature Growth of Single-Walled Carbon Nanotubes (SWNTs) from Monometallic Catalysts

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Small diameter single-walled carbon nanotubes (SWNTs) are regarded as potential building blocks in nanoelectronics. Obtaining (SWNTs) with narrow (n,m) chirality distribution are highly desirable since the electronic properties of SWNTs strongly depend on their diameter and chirality. Herein, we report the growth of small diameter SWNTs from cobalt catalysts deposited on conventional supports (SiO2, MgO) by atomic layer deposition (ALD). Various techniques were employed to analyze both the catalysts and SWNTs: Temperature Programmed Reduction (TPR), Raman, Absorption and Fluorescence Spectroscopy, Scanning electron microscope (SEM), ultra-high resolution transmission electron microscope ((Jeol JEM-2200FS double Cs corrector TEM). TEM has convinced that nanoparticles with diameters 2 to 4 nm were deposited onto different substrates by ALD. It was shown in Fig. a that high density SWNTs with high quality have grown successfully from the catalyst on silica substrate even at 550 °C. SWNTs diameters mainly range from 0.7 nm to 0.9 nm. UV-vis-NIR spectra of SWNTs produced at different temperatures are shown in Fig. b. Decreasing the reaction temperature leads to a progressive narrowing of the diameter distribution, this result is coincided with Raman spectra, photoluminescence intensity maps. Meanwhile, the mechanism for successful growth of SWNTs on various substrates, especially on MgO at low temperature has been provided.

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### Chiral Selective Nanotube Growth Using a Custom-Built Rapid Experimentation System

**Tonya Cherukuri**, *National Research Council Associate - Materials and Manufacturing Directorate, Air Force Research Laboratory* | **Rahul Rao**, *National Research Council Associate - Materials and Manufacturing Directorate, Air Force Research Laboratory* | **David Liptak**, *UES, Inc, Materials and Manufacturing Directorate, Air Force Research Laboratory* | **Benji Maruyama**, *Materials and Manufacturing Directorate, Air Force Research Laboratory*

Raman and fluorescence spectroscopy of single-walled carbon nanotubes (SWCNTs) during growth provides insight into the complex mechansims that govern nanotube chirality. We have developed a unique system that incorporates a chemical vapor deposition nanotube growth chamber with micro-Raman and near-infrared (NIR) fluorescence spectrometers. Growth occurs when catalyst nanoparticles deposited on thermally isolated islands are irradiated with the micro-Raman excitation laser which also serves as a localized heat source. Growth kinetics are obtained from the Raman signal from individual or small numbers of nanotubes in situ. The intrinsic NIR emission spectrum is obtained immediately after growth to identify the (n,m) chiral species of semiconducting nanotubes resulting from each set of experimental parameters. Automated control of substrate temperature, position, feed gas composition, and chamber pressure enable rapid real-time exploration of SWCNT growth parameter space. This system allows for the rapid analysis of the chiral distribution and growth kinetics of individual nanotubes while precisely tailoring experimental growth parameters toward a specific chirality.

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### An approach for defect healing in carbon structures: a tight-binding Monte Carlo study

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Carbon nanotubes and graphene are promising materials of remarkable mechanical and electronic properties that should give rise in the near future to revolutionary technologies. As of today, the mechanisms of germination and growth of the nano-objects are still very much misunderstood. Likewise, the selective and controlled growth of carbon nanotubes is currently unachievable. At atomic scale, several theoretical models of the nucleation mechanism exist. However, whether the employed method is empirical, semi-empirical or ab initio, all of the final configurations are plagued by a high concentration of defects. It is therefore, the aim of the present work to investigate how to heal these structures in order to correctly identify their chirality. We have at our disposal a semi-empirical model implemented into a Monte-Carlo code that enables us to study the effects of the temperature on graphitic structures grown by grand canonical Monte Carlo simulations [1]. We shall likewise investigate the role that catalysing metal plays in the nucleation and growth of graphitic structures. [1] H. Amara et al, PRB 79, 014109 (2009)

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### Synthesis of N-doped carbon nanotube arrays

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N-doped carbon nanotubes (CNT) arrays were directly synthesized on a substrate in a 2-in. quartz tube reactor horizontally inserted into a tube furnace using a chemical vapor deposition method. The carbon and nitrogen source used is acetonitrile. The catalyst used is ferrocene. In a typical experiment, the furnace is heated to a fixed temperature under a gas flow of 500 sccm Ar and 100 sccm H2. Then, the mixed ferrocene/acetonitrile is added to the reactor using a syringe pump (as shown in Fig.2) at a controlled rate. The N-doped CNT arrays started to grow on the substrate put in the furnace. After the growth, the supply of the ferrocene/acetonitrile mixture is stopped and the furnace is cooled down to room temperature. The morphology, composition, and micro-structure of N-doped CNT arrays were characterized with scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive X-ray (EDX) analysis.

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### In situ Raman spectroscopy as a precision probe of nanotube evolution during chemical vapor deposition

**Andrew Li-Pook-Than**, *University of Ottawa* | **Jacques Lefebvre**, *National Research Council of Canada, Institute for Microstructural Sciences* | **Paul Finnie**, *National Research Council of Canada, Institute for Microstructural Sciences*

In order to better understand growth and ultimately produce improved material, there is increasing interest in precisely tracking the evolution of carbon nanotube ensembles during synthesis. In this study, in situ Raman spectroscopy is used to study the CVD growth evolution of CNTs, grown using an ethanol precursor on cobalt catalyst with and without alumina support. The growth of three types of Raman bands, namely the G, D, and RBM bands, are tracked with time. Over a significant range of temperatures, close tracking between individual RBMs and between the RBMs and G band imply that the CNT diameter distribution is determined at growth onset and does not change over time. Similarly, close tracking between the G and D bands indicate that CNT crystallinity remains relatively constant throughout growth. A four step growth curve is observed for all bands, with distinct incubation, acceleration, linear, and termination stages. The growth rates of each stage are found to decrease with increasing growth temperature, suggesting the effect of parasitic reactions. Characteristic energy scales are extracted from each stage at each growth temperature. Studies such as this are promising routes for advancing our comprehension of nanotube growth processes.

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### Mossbauer Spectroscopy of residual iron in carbon nanotubes produced by camphor/ferrocene mixtures and purified by thermal annealing under vacuum

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**Marcos Massi**, *Instituto Tecnológico de Aeronáutica*

The most efficient way to eliminate iron from multi-walled carbon nanotube (MWCNT) powder is by annealing under vacuum using high temperatures. Beside iron evaporation, this kind of treatment brings improvement on graphitic ordering of tube wall. However very small quantities of iron (less than 1% in weight of carbon nanotubes) can be detected by Mossbauer spectroscopy. Hence, a study of iron phases present in as-grown MWCNT and MWCNT treated at high temperatures will be shown in this work. The MWCNT powder was obtained by pyrolysis of camphor mixed with ferrocene (16%), at 850oC under atmospheric pressure by 2h. The powder passed by thermal annealing under vacuum at temperature ranging from1500 to 1800oC during 1-2h The as-grown and purified MWCNT were analyzed by transmission electron microscopy (TEM), X-ray diffraction, thermogravimetric analysis and Mossbauer spectroscopy.

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### Role of plasma activation in the kinetics of CNT growth in PECVD process

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The work presents kinetic modeling of the effect of acceleration for the growth kinetics of carbon nanotubes by hydrocarbon gas mixture modification with plasma discharge. The plasma activation creates active species in hydrocarbon gas mixture, which can easily adsorb and dissociate on the catalyst surface. So plasma treatment of the gas mixture in the CVD process allows to increase the carbon supply rate by a few orders of magnitude compared to than in thermal CVD process. On the other hand, plasma can also provide etching of carbon species from the catalyst surface. To correctly reproduce both of these effects of plasma, the kinetic model of growth of carbon nanotubes is developed based on first-principles analysis of heterogeneous processes on the catalyst surface and detailed kinetics of gas phase chemistry. The model is used to compare the growth rates of carbon nanotubes in thermal and plasma-enhanced CVD processes and to determine critical gas pressures, at which CNT growth switches from the adsorption limitation to the limitation by reaction and diffusion on the catalyst.

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### Carbon Nanotube Fibres from Natural Gas: An Economic and Scalable Route to Carbon Nanotube Fibre Production

**Fiona Smail**, *Department of Materials Science and Metallurgy, University of Cambridge* | **Juan Vilatela** | **Krzysztof Koziol** | **Rajyashree Sundaram** | **Rupesh Khare** | **Jing Qiu** | **Alan Windle**

The improving mechanical properties associated with carbon-nanotube fibres continue to capture the imagination of scientists, engineers and technology developers worldwide. However, it is acknowledged that a route is required to make bulk quantities of fibre for full-scale applications-testing purposes. One of the most promising routes under development is via chemical vapour deposition, where a carbon source is cracked on the surface of iron nanoparticles in a continuously flowing stream of carrier gas. In The Cambridge Process the grown nanotubes agglomerate in the reactor to form an annular sock which is continuously drawn out of the reactor onto a spindle turning at up to 70 m/min, resulting in kilometres of fibre. Many different carbon sources have been researched as precursors for individual carbon nanotubes but fewer have been studied with respect to nanotube-fibre production and to date the identification of an economical, scaleable carbon source for sustainable bulk fibre production has attracted little attention. Natural gas is a readily-available, relatively inexpensive feedstock and the paper presents the first studies of fibre from this source. The mechanical and structural properties of the fibres are compared with those from other carbon sources made in the same process and the effects of dosing the main feedstock with other carbon precursors are also shown. The carbon yield for a range of feedstocks is compared with that of natural gas and the economic case, resting on the degree of carbon capture and low cost of the feedstock as compared to other carbon sources, is also presented

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### TEM-EELS analysis of catalyst metals for high-density carbon nanotube growth

**Akio Kawabata**, *MIRAI-Slete; Fujitsu Ltd.* | **Haruhisa Nakano**, *MIRAI-Slete* | **Tomo Murakai**, *MIRAI-Slete* | **Tomomi Daidou**, *MIRAI-Slete* | **Motonobu Sato**, *MIRAI-Slete; Fujitsu Ltd.* | **Takashi Hyakushima**, *MIRAI-Slete* | **Shintaro Sato**, *MIRAI-Slete; Fujitsu Ltd.* | **Mizuhisa Nihei**, *MIRAI-Slete; Fujitsu Ltd.* | **Yuji Awano**, *MIRAI-Slete* | **Naoki Yokoyama**, *Fujitsu Laboratories Ltd.*

In our research, we tried to use bundles of carbon nanotubes (CNTs) as low-resistivity vertical via interconnects for high-performance LSIs. To lower the resistance of CNT vias, we need to increase the site density of CNTs in a CNT bundle. We have already reported on the high-density CNT growth of more than 1012 tubes/cm2 achieved by optimizing catalyst metals [1]. In this study, we analyzed the metal structure of the activated catalyst after the CNT growth by taking cross-sectional TEM-EELS measurements. CNTs were synthesized by the thermal chemical vapor deposition (CVD) method. A Co catalyst was deposited on a TiN contact layer/TaN barrier layer/Cu film. In this experiment, the thicknesses of the Co and TiN were 1.0 nm and 0.5 nm, respectively. The source gas for CVD was C2H2 diluted by Ar, and the substrate temperature was 450°C. From the TEM-EELS measurements, we found that the Co and Ti overlaid each other in the activated catalyst. On the other hand, the Co and Ti were almost separated in the catalyst that produced almost no CNT growth. We speculated that the Ti that wrapped or interacted with Co catalyst helped activate the growth of CNTs. Acknowledgements: This work was completed as part of the MIRAI Project supported by NEDO. [1] A. Kawabata et al., NT09.

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### Water based PECVD process for the growth of oriented and patterned carbon nanotubes

**Aurelien Gohier**, *LPICM, Ecole Polytechnique, France* | **Zhanbing He**, *LPICM, Ecole Polytechnique, Palaiseau, France* | **Pierre Legagneux**, *Nanocarb, Thales R&T, France* | **Jean-Luc Maurice**, *LPICM, Ecole Polytechnique, France* | **Costel Cojocaru**, *LPICM, Ecole Polytechnique, Palaiseau, France*

Since the study reported by Hata et al. [1], the use of water as weak oxidizer in CVD process has attracted great attention for the growth of vertically-aligned ultra-long carbon nanotubes. Notably, it has been shown that very low concentration of water vapour (<1 vol.%) can selectively etch amorphous carbon while preventing the catalyst from its deactivation. Although the beneficial aspects of water have been widely studied for CVD process [2], very few groups have investigated its impact on the growth of CNTs by plasma assisted CVD [3]. Here, we demonstrate that water can be used in large amount to grow oriented CNTs by plasma enhanced CVD. A direct-current plasma set-up was used to study the growth kinetics of CNTs using water/hydrocarbon mixture. Such a process is shown to achieve CNT growth at temperature as low as 450°C without any amorphous carbon deposition. We have also studied the ability of the water-based process to grow patterned and individualized CNTs. Two paths for the preparation of patterned catalyst were investigated: i) standard lithography ii) ink-jet printing. The use of the resulting vertically-aligned CNTs as field emitters has been demonstrated and will be discussed. [1] K. Hata et al. Science 306 (2004) 1362 [2] G. Zhang PNAS 102 (2005) 16141 [3] M. Meyyappan J. Phys. D 42 (2009) 213001

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### Surface growth of carbon nanotubes: entanglement versus vertical-alignment by manipulating the catalyst-support interactions

**Santiago Esconjauregui**, *University Of Cambridge* | **B Bayer**, *University Of Cambridge* | **M Fouquet**, *University Of Cambridge* | **J Robertson**, *University Of Cambridge*

Engineering of the catalyst-support interface allows fine control of the surface growth of carbon nanotubes (CNTs) in terms of entanglement versus vertical-alignment. Oxidising pretreatments of silica coated with Ni, Co, and Fe result in high-density vertically-aligned CNTs. X-ray photoelectron spectroscopy reveals strong catalyst-support interactions at the silica-metal interface, which restricts catalyst mobility and promotes base growth and CNT alignment. Conversely, reducing environments result in weak silica-metal interactions, with nanoparticles of high mobility that sinter at high temperatures and promote entangled CNTs only.

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### High efficiency growth of individual 20 cm long DWNTs/TWNTs by water assisted methane-CVD

**Weizhong Qian**, *Tsinghua University* | **Qian Wen**, *Tsinghua University* | **Jinqi Nie**, *Tsinghua University* | **Rufan Zhang**, *Tsinghua University* | **Yuran Wang**, *Tsinghua University* | **Fei Wei**, *Tsinghua University*

We proposed gas flow directed CH4- CVD to grow centimeters long CNTs with certain sections possessing the same chiral angle and the same (n,m)index. Adding water in this system helped to increase the growth rate of long CNTs from 20 μm/s to 80~90 μm/s. Raman characterization showed the long tubes had a nearly perfect structure. By comparing the Si substrate,the role of water was to remove the amorphous carbon around the catalyst site in CVD process. TEM characterizations suggested the distribution of diameter and number of walls of CNTs is a little bit changed by adding water. At last, it was shown that these long tubes can be grown without the use of long Si substrates. Instead, many short Si and SiO2 substrates put together in line could be used. Thus, our results showed a highly efficient and cheap method for the large scale up preparation of centimeters-long CNTs.

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### Effect of alcohol precursors on the purity of CNT fibres synthesised by CVD

**Rajyashree Sundaram**, *University Of Cambridge* | **Krzysztof Koziol**, *University Of Cambridge* | **Alan Windle**, *University Of Cambridge*

Synthesis of pristine carbon nanotubes (CNTs) by chemical vapour deposition (CVD) and its direct assembly into macroscopic entities such as fibres and films is attractive and desirable for a wide range of applications. CVD involves the decomposition of gaseous or volatile carbon compounds in the presence of transition metal catalyst nanoparticles (either formed in situ or prior to the reaction), which nucleate CNT growth under reaction temperatures ranging from 600°C to over 1000°C. The product characteristics – composition and yield, can be finely controlled by adjusting reaction parameters and the pyrolysis chemistry of the reactants – carbon precursors in the presence of a catalyst and promoter. A variety of carbon sources including hydrocarbons (aromatic and aliphatic), alcohols, CO have been explored under diverse conditions. A discussion on our attempts to explore the synthesis parameters, which could result in the formation of high quality nanotubes in fibres obtained from an aerogel-based CVD synthesis developed in the University of Cambridge, will be presented. The extent of presence of extraneous materials, relative carbon conversion yields and iron utilisation of the various alcohols will be dealt with, in the context of the interplay of pyrolysis chemistry and the precursor solution injection conditions. The role of 'C:O ratio' in producing CNTs of enhanced purities and its effect on the lifetime of the catalyst will be discussed.

## Poster Board | 292

### Towards Integration of Parallel CNT Growth Techniques with Si Technology

**Hari Pathangi Sriraman**, *imec, Belgium; Department of Electrical Engineering, Katholieke Universiteit Leuven, Belgium* | **Nicolo' Chiodarelli**, *imec, Belgium; Department of Electrical Engineering, Katholieke Universiteit Leuven, Belgium* | **Nalin Rupesinghe**, *Aixtron Ltd., Cambridge, United Kingdom* | **Ken Teo**, *Aixtron Ltd., Cambridge, United Kingdom* | **Guido Groeseneken**, *imec, Belgium; Department of Electrical Engineering, Katholieke Universiteit Leuven, Belgium* | **Ann Witvrouw**, *imec, Belgium* | **Philippe M. Vereecken**, *imec, Belgium; Centre for Surface Chemistry and Catalysis, Katholieke Universiteit Leuven, Belgium*

The unique physics of CNTs and their exceptional material properties have resulted in numerous breakthroughs in the recent past. In spite of this, the destiny of CNTs as future devices at a commercial level is uncertain due to the lack of control in their fabrication. Therefore, methods, preferably compatible with Si micro-fabrication techniques, which can control the on-chip CNT density, hold the key to this problem. We describe the development of a process flow involving controlled Ni catalyst deposition on titanium nitride (TiN) by electrochemical deposition (ECD). TiN was chosen as the CNT growth surface as it is widely used in IC fabrication. Also, ECD can be used for site-selective catalyst placement, in contrast to the commonly used thermal evaporation or drop cast methods, and is compatible with Si back-end of line processing. RBS and SEM were used to calibrate the Ni ECD from an aqueous solution of nickel sulphate and sodium citrate. CNT growth was successfully performed from the Ni catalyst on blanket TiN by thermal CVD at 570°C. Further efforts are being pursued to grow CNTs at lower temperatures, more suitable for above-IC integration (~450°C). Using a Si compatible scheme, TiN electrode structures were processed on 200mm wafers as templates for CNT device fabrication towards NEMS and sensor applications. The electrodes design allows for wafer-scale deposition of the growth catalyst in parallel at specific sites. The scalability of our process and the wafer-scale batch fabrication techniques used are key steps towards commercial relevance of CNT applications.

## Poster Board | 293

### Effect of pressure and temperature on growth and properties of different nanostructures produced by High Pressure CVD

**Albrecht Leonhardt**, *Leibniz Institute For Solid State And Material Research* | **Vyacheslav O. Khavrus**, *Leibniz Institute For Solid State And Material Research* | **Eslam M.M. Ibrahim**, *Leibniz Institute For Solid State And Material Research* | **Ahmed A. M. El-Gendy**, *Leibniz Institute For Solid State And Material Research* | **Silke Hampel**, *Leibniz Institute For Solid State And Material Research*

Considerable efforts have been made in the recent years to develop methods for selective synthesis of various shaped carbon nanomaterials (SCNMs) such as carbon-protected nanoparticles (NPs), single- and multi-walled carbon nanotubes (SWCNTs, MWCNTs). Their preferential formation is a big challenge that needs to be solved for the future applications. During last decade various SCNMs have attracted an increasing interest, due to many potential applications in drug delivery, chemical technology, magnetic data storage devices, and nanoscale electronics. Particularly, carbon-encapsulated metal nanoparticles are promising candidates for various biomedical applications. For the synthesis of SCNMs, chemical catalytic vapor deposition method is a strong manufacturing route due to the ability of producing bulk amount of nanomaterial on a large-scale and controlling their structure more easily compared to other synthesis methods. In our work, we used the high-pressure chemical vapor deposition (HiPCVD) system which operates in wide range of pressure (1…40 bar). In our work we report on the synthesis of different types of SCNMs. We have developed a simple and effective method for preferential fabrication of undoped and nitrogen-doped SWCNTs, carbon-encapsulated metal NPs (Fe, Co, Ni) or MWCNTs in one and the same equipment. Conditions of formation such nanostructures were determined, their morphologies and properties were characterized by different methods (Scanning and transmission electron microscopy, X-ray photoelectron and Raman spectroscopy, alternating gradient magnetometry).

## Poster Board | 297

### Large-scale Synthesis of Single-walled Carbon Nanotubes from Biorenewable Carbon Resources

**Keun Su Kim**, *National Research Council Of Canada* | **Christopher Kingston**, *National Research Council Of Canada* | **Dean Ruth**, *National Research Council Of Canada* | **Michelle Nagy**, *National Research Council Of Canada* | **Stephane Denommee**, *National Research Council Of Canada* | **Michael Barnes**, *National Research Council Of Canada* | **Orson Bourne**, *National Research Council Of Canada* | **Benoit Simard**, *National Research Council Of Canada*

Thanks to their exceptional physic-chemical properties, single-walled carbon nanotubes (SWCNTs) are considered as the ultimate material in diverse fields. Thus there have been tremendous efforts to develop economical production methods for those materials at large scales, and many processes are now well established. However, as the increasing concern on the environment has been a formidable challenge to our society, we need more sustainable routes to produce SWCNTs. In conventional processes, feedstock materials mainly rely on hydrocarbons or carbon blacks which are not renewable. In this experimental work, we report a development of an eco-friendly process for the large-scale production of SWCNTs that uses biochar as a feedstock material. In this new process, SWCNTs are produced from direct evaporation of biochar in the plasma jet generated from an induction plasma torch, and it has been successfully demonstrated that biochar would serve as a good carbon precursor for SWCNT production. We will present our recent results focusing on the effects of pre-treatment of biochar and plasma operating conditions on the quality of the SWCNTs produced.

## 10:01-11:30 Poster Session 3

### Poster Board | 3

### Chemisorption of Hydrogen on Graphite (0001): Spin-Polarized Density-Functional Tight-Binding Molecular Dynamics Simulations Using G2MS-Derived C-H Parameters

**Ying Wang**, *Institute for Advanced Research and Department of Chemistry, Nagoya University* | **Atsushi Ito**, *National Institute for Fusion Science, Toki* | **Hiroaki Nakamura**, *National Institute for Fusion Science, Toki* | **Keiji Morokuma**, *Fukui Institute for Fundamental Chemistry, Kyoto University* | **Stephan Irle**, *Institute for Advanced Research and Department of Chemistry, Nagoya University*

Original self-consistent-charge density-functional tight-binding (SCC-DFTB) potential energy curves (PECs) for the hydrogen chemisorption on a central carbon atom of pyrene and coronene molecules are qualitatively wrong compared to those predicted by DFT (B3LYP/cc-pVDZ), ab initio (RCCSD(T)/cc-pVDZ), and G2MS levels of theory. First principles and ab initio methods of PECs for both pyrene and coronene species feature a barrier of ~0.4 eV and a potential well of ~-0.5 eV. Spin-polarized SCC-DFTB (SDFTB) performs better regarding the well depth but the barrier height is too low with <0.1eV. We modified the C-H repulsive parameter function to adjust the SDFTB interaction energy to the G2MS PEC of coronene, and are now able to obtain perfect agreement between the resulting SDFTB with improved Erep(C-H) (SDFTB*) and G2MS. Using SDFTB* we performed microcanonical MD simulations of chemical sputtering of individual hydrogen atom and graphite (0001) with 160 carbon atoms in a nearly square planar unit cell. Following previous modified reactive empirical bond order (REBO) semiclassical molecular mechanics simulations, we probed H atoms between 0.1 and 100 eV by supplying corresponding initial vertical velocities on the hydrogen atoms, which were placed in randomly over the target graphite surface up to 200 trajectories per incident energy. Adsorption, reflection, and penetration are observed. Since SDFTB* features a much shallower adsorption well than the modified REBO potential (-4.8eV), the absorption yield is different. In addition, SDFTB*/MD penetration occurs earlier compared to REBO, which indicates that lower graphite layers should be affected by lower hydrogen compared to the REBO results.

### Poster Board | 6

### Edge Magneto-Fingerprints in Disordered Graphene Nanoribbons

**Jean-marie Poumirol**, *LNCMI - CNRS, Université de Toulouse, France* | **Alessandro Cresti**, *CEA, LETI, MINATEC, France* | **Stephan Roche**, *CIN2 (CSIC-ICN), Campus UAB, Spain* | **Rebeca Ribeiro**, *LNCMI - CNRS, Université de Toulouse, France* | **Walter Escoffier**, *LNCMI - CNRS, Université de Toulouse, France* | **Michel Goiran**, *LNCMI - CNRS, Université de Toulouse, France* | **Xinran Wang**, *Department of Chemistry and Laboratory of Advanced Materials, Stanford University, USA* | **Xiaolin Li** *Department of Chemistry and Laboratory of Advanced Materials, Stanford University, USA* | **Hongjie Dai**, *Department of Chemistry and Laboratory of Advanced Materials, Stanford University, USA* | **Bertrand Raquet**, *LNCMI - CNRS, Université de Toulouse, France*

The control of the current flow in graphene nanoribbons (GNRs) constitutes a fascinating challenge for the future of carbon-based electronic devices. However, non-perfect edges, bulk vacancies, charge trapped in the oxide or structural deformations are potential sources of backscattering. Their respective contribution remains debated and seems to be sample dependent. This work presents compelling evidences of the 1D transport character in the first generation of chemically derived GNRs with smooth edges, and the possibility of tuning backscattering effects by means of an external magnetic field [1]. Bandstructure calculations allow some assignment of the measured gate-dependent conductance modulations to the underlying van Hove singularities, and hence some estimation of the likely ribbon edge symmetry. The application of perpendicular high magnetic field further induces a marked enhancement of the conductance, irrespective of the applied gate voltage and in large contrast to the magnetofingerprints of graphene flakes. Close to the charge neutrality point, the measured large positive magnetoconductance is attributed to the formation of the first Landau state, responsible for the closing of the energy gap and of a marked reduction of backscattering processes. Landauer-Buttiker conductance simulations convincingly support the scenario of an entangled interplay between the magnetic bands formation and a disorder-induced interband scattering suppression. Both smooth edge disorder and long range Coulomb scatters yield similar conclusions. Finally, a comparative magneto-transport study between chemically derived GNRs and patterned GNR by oxygen plasma reactive ion etching will be addressed. [1] J-M Poumirol et al., arXiv:1002.4571

### Poster Board | 9

### Photocatalytic Paper-cutting for Graphene Electronics

**Liming Zhang**, *Peking University* | **Shuo Diao**, *Peking University* | **Jing Kong**, *Massachusetts, Institute of Technology* | **Zhongfan Liu**, *Peking University*

Due to the excellent carrier transport properties and potentials for future applications in nanoelectronics, graphene has been paid great attention since its isolation in 2004. Previous calculations have shown that, depending on the size, geometry, crystallographic orientations and edge structure, graphene can display a variety of electronic properties. So far, several ways have been reported on graphene cutting, including e-beam lithography, chemical stripping, catalytic hydrogenation and scanning tunneling microscope lithography. We report here a novel method to tailor graphene sheets into desired shapes and sizes in ambient environment. Nano-scissors are considered to be active oxygen species produced in photocatalytic reaction. Under UV irradiation, hole/electron pairs separate on the surface of titanium dioxide (TiO2) and produce active oxygen species, e.g. hydroxyl radicals(HO•), superoxide ions(O2-) and hydroperoxyl radicals (HOO•) through reactions with H2O and O2 in air. These active species decompose and cut the sheets. Graphene with different shapes are thus obtained by using patterned TiO2 mask. This method is feasible for graphene produced by different methods and on arbitrary substrates. We also found the cutting rate is extremely depending on the humidity and oxygen concentration of the surroundings. The edge of graphene after photocatalytic cutting is comparable to that of EBL. Through investigation on HOPG surface, it is found that the photocatalytic cutting was initiated at defects preferentially in an anisotropic feature, with the in-plane reaction being of one order faster than vertical direction. All-carbon FETs in which graphene serves as electrical contacts and SWNTs as conduction channels are also demonstrated.

### Poster Board | 12

### Low-temperature graphene synthesis and its application to transparent flexible conductive films

**Byeong-Joo Lee**, *Kangwon Natioinal University* | **Se-Rin Park**, *Korea Research Institute of Chemical Technology* | **Han-Young Yu**, *Electronics and Telecommunications Research Institute* | **Jeong-O Lee**, *Korea Research Institute of Chemical Technology* | **Goo-Hwan Jeong**, *Kangwon Natioinal University*

Graphene has been attracting much attention owing to its fascinating mechanical, electronic and optical properties. Fundamental and application researches are now intensively undergoing to realize their potential uses. Several approaches on graphene synthesis have been developed including mechanical and chemical exfoliation methods, thermal chemical vapor deposition (TCVD), graphitization of SiC surfaces and reduction of graphene oxides. The TCVD method is prevailing for large scale synthesis of graphene with high uniformity of graphene thickness. However, high temperature process is inevitable for thermal decomposition of carbon containing gases. Lowering the synthesis temperature is definitely beneficial to expand their accessibility in both scientific and industrial fields. As for application, graphene can be applied to not only functional devices such as sensors and memories but also transparent and flexible conducting film which can be substituted for ITO in various fields. In this study, we present low temperature synthesis of graphene using hybrid chemical vapor deposition (HCVD) system which is consisted of plasma CVD using radio frequency for enhanced dissociation of feeding gas and thermal CVD. As for synthesis, E-beam deposited Ni film and Cu foils were used as substrates and methane was carbon feedstocks. As a result, we confirm that few layer graphene was synthesized around 600°C. After synthesis, as-grown films could also be transferred to silicon oxide covered wafer and transparent polymer substrate for both facile characterization and various application. As-grown and transferred films were analyzes with optical microscopy, Raman spectroscope, atomic force microscopy, scanning electron microscopy and transmission microscopy.

## Poster Board | 15

### Fabrication of Conductive Poly(3,4-ethylenedioxythiophene) and Graphene Composite Films by a Layer-By-Layer Assembly Method

**Ki Seok Choi**, *KAIST* | **Fei Liu**, *KAIST* | **Tae Seok Seo**, *KAIST*

Poly(3,4-ethylenedioxythiophene) (PEDOT)-based thin film has relatively high conductivity, flexibility and transmittance. However, the improvement for mechanical strength and enhanced conductivity is still required to be adatped for commerical applications. Graphene, a one-atom-thick planar sheet of sp2-bonded carbon atoms is considered as an ideal nanocomposite material for these purposes. In this study, we have developed a PEDOT and graphene composite films, two layered graphene/PEDOT and three layered graphene/PEDOT/graphene, by using a layer-by-layer method. The conductivity of 32 nm-thick PEDOT film was improved more than twice by graphene deposition, while the high transmittance of the composite film was maintained. The mechanical strength of the PEDOT and graphene composite film shows 6-fold enhancement over the pristine PEDOT film. Due to the contribution of graphene layer for the improved mechanical strength, the 44 nm-thick graphene/PEDOT/graphene could be obtained as a free standing film by delaminating the graphene layer from the glass substrate under a weak base solution. These results imply that the graphene not only improves the conductivity and mechanical strength of PEDOT film, but also enables to produce a free standing film which could find a variety of applications in the fields of organic electronic, sensors and optoelectronics.

## Poster Board | 18

### Highly Conductive Graphene Film Electrode for Ultrasensitive Pathogen Detection

**Fei Liu**, *KAIST* | **Tae Seok Seo**, *KAIST*

Graphene film based biosensor system was presented for performing pathogenic virus detection. Free standing graphene oxide (GO) film was generated by a centrifugal evaporation in a speed vacuum concentrator, and a thermal annealing process at 800 oC with H2/Ar flow has converted GO film to highly conductive graphene films. The reduced graphene film was used as a working electrode for an electrochemical biosensor, in which the graphene film was attached on the gold electrode and fixed with a polydimethylsiloxane (PDMS) chamber, and a Pt wire and a Ag/AgCl electrode were employed as a counter electrode and a reference electrode, respectively. The surface of graphene film was modified with pyrene derivatives, and then linked with virus-specific antibodies. The target cell, Rotavirus, was captured on the graphene film through antibody-antigen interaction, and the entire process was monitored by cyclic voltammetric response. While 10^5 cfu/mL concentration of input cells showed ca. 30% sensitivity, the 10^2 cfu/mL concentration of input cells was detected with ca. 7% sensitivity in the cyclic voltammograms, demonstrating graphene based ultrasensitive pathogen detection.

## Poster Board | 24

### Alcohol CVD synthesis of single-layer graphenes using flash cooling

**Yasumitsu Miyata**, *Department of Chemistry, Nagoya University, Japan* | **Keiichi Kamon**, *Department of Chemistry, Nagoya University, Japan* | **Ryo Kitaura**, *Department of Chemistry, Nagoya University, Japan* | **Masamichi Yoshimura**, *Toyota Technological Institute* | **Hisanori Shinohara**, *Department of Chemistry, Nagoya University, Japan*

We report the facile synthesis of single-layer graphenes from alcohol using, what we-call, gflash coolingh after chemical vapor deposition (CVD). The graphenes were synthesized on a nickel (Ni) substrate using ethanol as a carbon source. The synthesized single-layer graphenes so synthesized are high-quality and several micrometers in grain size as revealed by Raman spectroscopy. Interestingly, the graphenes have never been observed for naturally-cooled Ni substrates. This means that the synthesized graphenes were decomposed during the natural cooling and that the flash cooling does not lead to this decomposition. We, therefore, conclude that carbon absorption on the Ni surface consist mainly of the following two different processes: the carbon dissolution into the Ni and the direct formation of graphenes on the Ni surface. The present results show a promising single-layer graphene synthesis in high quality on various metal substrates.

## Poster Board | 30

### Molecular dynamics and kinetic modeling of phonon transport in defective carbon nanostructures

**Andrey Knizhnik**, *Kintech Lab Ltd, Moscow, Russia* | **Inna Iskandarova**, *Kintech Lab Ltd, Moscow, Russia* | **Dmitry Krasikov**, *Kintech Lab Ltd, Moscow, Russia* | **Alexander Eletskii**, *Kintech Lab Ltd, Moscow, Russia* | **Boris Potapkin**, *Kintech Lab Ltd, Moscow, Russia* | **Vinayak Tilak**, *GE Global Research, Niskayuna, USA* | **Kamala Raghavan**, *GE Global Research, Bangalore, India*

Low dimensional carbon nanostructures, such as carbon nanotubes, graphene, possess unique physical properties, in particular, high thermal conductivity. These unique physical properties depend strongly on the structural and compositional characteristics of nanostructures. Atomistic methods, such as equilibrium and non-equilibrium molecular dynamics, are widely used to investigate dependence of thermal conductivity on the structure of the nanomaterial, in particular on the number and nature of defects. However, atomistic methods have severe drawbacks in considering real nanostructures due to the spatial and temporal limitation. At the same time, available macroscopic methods, such as kinetic Boltzmann equation, can overcome size limitations of atomistic methods, but cannot predict accurately scattering properties of structural and compositional defects.
In this work we present the results of combination of molecular dynamics method for calculation of thermal conductivity with macroscopic method based on Boltzmann transport equation. We made direct comparison of these two methods using parameters of macroscopic model derived from the results of atomistic simulations of intermediate-size systems. We also performed investigation of influence of point defects on thermal transport in graphene using molecular dynamics and Boltzmann transport equation model. While systems with super micron-scale cannot be considered now directly with molecular dynamics methods, we were able to describe thermal properties of these systems using combined approach. Based on the results of the proposed approach we investigate the effect of different types of defects on thermal conductivity and determine the critical fraction of point defects in the carbon nanostructures as a function of their length.

## Poster Board | 33

### Structural, magnetic, and conductance properties of doped nanoribbons from first-principles.

**Zachary Barnett**, *University Of Tennessee; Oak Ridge National Laboratory* | **Eduardo Cruz-Silva**, *Oak Ridge National Laboratory* | **Bobby Sumpter**, *Oak Ridge National Laboratory* | **Vincent Meunier**, *Oak Ridge National Laboratory*

In recent years, the study of electron transport within graphene and graphitic nanoribbons (GNRs) has increased significantly due to the promise of their tunable properties resulting in novel electromagnetic devices. One key aspect toward realizing these promises is to understand the effects of doping on the ribbons' electronic properties. Using density functional theory calculations, we have performed a detailed study of the energetics, electronic band structures, and conductance properties in a 1.23 nm-wide zigzag nanoribbon and an 1.39 nm-wide armchair nanoribbon substitutionally doped with a single boron, nitrogen, or phosphorus atom in positions ranging from the edge to the center of the ribbon. Our results show that the structures with the dopant on the ribbon edge possess the lowest formation energy, with the notable exception of the boron-doped armchair ribbon, which has the lowest formation energy in the position just next to the edge. Additionally, we observe that the boron-doped zigzag nanoribbons exhibit spin-dependent donor-like states when the dopant is on the ribbon edge, and acceptor states as the dopant moves toward the ribbon center. Nitrogen doped zigzag nanoribbons show the opposite effect, and phosphorus doped zigzag nanoribbons show both donor-like and acceptor-like states. The band structure and local density of states of these ribbons indicate that dips in conductance occur from either the presence of a localized state or the opening of mini band-gaps at a particular energy. The presence of this spin-dependent behavior may be useful in creating spintronic devices from GNRs.

## Poster Board | 36

### Tunable bandgap versus electron localization in hydrogenated quasi-free-standing graphene

**Danny Haberer**, *IFW Dresden, Germany* | **Denis Vyalikh**, *Institut fuer Festkoerperphysik, TU Dresden, Germany* | **Luca Petaccia**, *SincrotroneTriesteS.C.p.A., Italy* | **Simone Taioli**, *FBK-IRST Center for Materials and Microsystems, Italy; The European Center for Theoretical Studies in Nuclear Physics and Related Areas (ECT), Italy; Department of Physics, University of Trento, Italy* | **Balazs Dora**, *Department of Physics, Budapest University of Technology and Economics, Hungary* | **Mani Farjam**, *Institute for Research in Fundamental Sciences (IPM), Iran* | **Thomas Pichler**, *Faculty of Physics, University of Vienna, Austria* | **Stefano Simonucci**, *FBK-IRST Center for Materials and Microsystems, Italy* | **Martin Knupfer**, *IFW Dresden, Germany* | **Bernd Buechner**, *IFW Dresden, Germany* | **Alexander Grueneis**, *IFW Dresden, Germany; Faculty of Physics, University of Vienna, Austria*

Regarding the device applications of graphene, chemical functionalization is one of the key strategies to tailor its electronic properties. We have carried out functionalization of CVD grown graphene monolayers with alkali and hydrogen atoms. This enables us to tune the energy bandgap as well as the electron concentration independently. The chemical bonding and the concentrations of the adsorbed atoms are determined with high accuracy using core level and x-ray absorption spectroscopies. Angle-resolved photoemission spectroscopy is employed to access the electron-phonon coupling constant and its dependence on doping level, wavevector direction and impurities. Furthermore, the metal insulator transition in graphene is discussed in terms of band insulator versus electron localization.

## Poster Board | 39

### Tomonaga-Luttinger liquid physics in gated bilayer graphene

**Matthew Killi**, *University of Toronto* | **Tzu-Chieh Wei**, *University of British Columbia* | **Ian Affleck**, *University of British Columbia* | **Arun Paramekanti**, *University of Toronto*

Electronically gated bilayer graphene behaves as a tunable gap semiconductor under a uniform interlayer bias Vg. Imposing a spatially varying bias, which changes polarity from -Vg to +Vg, leads to one dimensional (1D) chiral modes localized along the domain wall of the bias. Due to the broad transverse spread of their low-energy wavefunctions, we find that the dominant interaction between these 1D electrons is the forward scattering part of the Coulomb repulsion. Incorporating these interactions and the gate voltage dependence of the dispersion and wavefunctions, we find that these 1D modes behave as a strongly interacting Tomonaga-Luttinger liquid with three distinct mode velocities and a bias dependent Luttinger parameter, and discuss its experimental signatures.

## Poster Board | 42

### Resistive nonvolatile memory based on spin cast graphene oxide thin films

**Jong Yun Kim**, *Electronics and Telecommunications Research Institute (ETRI)* | **Hu Young Jeong**, *Electronics and Telecommunications Research Institute (ETRI)* | **Hong Kyw Choi**, *Electronics and Telecommunications Research Institute (ETRI); Department of Advanced Device Technology, University of Science and Technology (UST)* | **Sung-Yool Choi**, *Electronics and Telecommunications Research Institute (ETRI); Department of Advanced Device Technology, University of Science and Technology (UST)*

We present a novel solution-processible nonvolatile cross-point memory array based on graphene oxide (GO) thin film. GO is the oxygenated derivate of graphene usually prepared by chemical oxidation of naturally abundant graphite. Oxygen functional groups such as epoxide, hybroxyl, and carboxyl groups decorating the basal plane and edge endow GO with aqueous solubility. In this work, a facile and scalable process for trilayer device structure of Al/GO/Al is realized using uniform GO film prepared by spin casting. The trilayer GO device showed reliable and reproducible bipolar resistive switching (BRS) with an on/off ratio of ~100, a retention time of longer than 105, and switching voltages of ~2 V. The origin of such unique switching behavior was thoroughly investigated. High-resolution TEM and in situ x-ray photoemission spectroscopy (XPS) measurements verified that the oxygen functional groups decorating the GO sheets migrate into the top interface layer by redox reaction with top Al electrode. Based on the concrete experimental observation, the microscopic origin of BRS behavior is attributed to the reversible formation and disruption of local conductive filament at the top interface layer, which is induced by the reversible drift of negative charged oxygen functional ions upon set/reset processes.

## Poster Board | 45

### Synthesis of thin graphene layers on Ni surface by plasma-enhanced chemical vapor deposition

**Eunsung Kim**, *Department of Energy Science, Sungkyunkwan University* | **Ganghee Han**, *Department of Physics, Sungkyunkwan University* | **Hyunjin Shin**, *SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University* | **Seungjin Chae**, *SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University* | **Fethullah Gunes**, *SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University* | **Younghee Lee**, *Department of Energy Science, Sungkyunkwan University; Department of Physics, Sungkyunkwan University; SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University*

A two-dimensional single graphene layer has recently observed in the sphere of science by considerable interests. We have synthesized thin graphene layers using remote RF plasma-enhanced chemical vapor deposition on Ni surface. In the synthesis process, we supplied gas mixture of H2 and C2H4. Growth temperature, plasma power, treatment time, and gas mixing ratio were optimized to minimize the defects on graphene and maintain uniformity of the synthesized graphene layers. For the synthesis, sub tens of micrometer Ni film was used. Synthesized graphene layers was transferred on various substrates and characterized by optical microscope, Raman spectroscopy, field-emission scanning electron microscopy (FE-SEM), and atomic force microscopy (AFM).

## Poster Board | 51

### Ultrafast photoluminescence from graphene

**Chun Hung Lui**, *Columbia University, USA* | **Kin Fai Mak**, *Columbia University, USA* | **Jie Shan**, *Case Western Reserve University, USA* |

**Tony F. Heinz**, *Columbia University, USA*

Since graphene has no band gap, light emission is not expected from fully relaxed carriers. However, we observed strong light emission from monolayer graphene under excitation by ultrashort (30-fs) laser pulses. The emission spectrum was found to extend from the visible range to photon energy of 3.5 eV in the near UV, greatly exceeding that of the pump laser at 1.5 eV. Beside detailed measurements of the emission spectra for different pump fluences, we have also applied an ultrafast time-domain correlation technique in which light emission was measured as a function ofthe temporal separation between a pair of femtosecond excitation pulses. A dominant relaxation time of a few tens of femtoseconds was observed. Our results indicate that the unusual light emission process originates from non-equilibrium photoexcited charge carriers in graphene. Further analysis reveals strong carrier-carrier scattering processes and rapid electronic cooling through optical phonon emission in graphene on the sub-100fs time scale.

## Poster Board | 60

### Graphene and graphene decorated with metal nanoclusters investigation for routing electronic application

**Ivan Bobrinetskiy**, *Moscow Institute Of Electronic Technology (Technical University)* | **Vladimir Nevolin**, *Moscow Institute Of Electronic Technology (Technical University)* | **Semen Chervonobrodov**, *NanoCarbLab (www.nanocarblab.com)* | **Larisa Kvacheva**, *Institute of organoelement compound RAS* | **Sergey Abramchuk**, *Institute of organoelement compound RAS* | **Denis Levin**, *Moscow Institute Of Electronic Technology (Technical University)* | **Konstantin Gorshkov,** *Moscow Institute Of Electronic Technology (Technical University)*

The graphene and graphene decorated with metal nanoclusters were investigated with making use of high resolution microscopy (atomic force microscopy (AFM), transmission electron microscopy (TEM)) and high resolution focused ion-beam lithography in terms of electronic application. The graphene compounds, produced by NanoCarbLab, were investigated with making use of AFM. The samples dissolved in propanol or chloroform to make the colloid suspension. We have dissolved the problem of graphene coagulation when it was deposited on substrate surface (typically, silicon dioxide). In AFM-image the few-layered graphene lateral sizes varied from 1 to several tens of micrometers. The results were the same in TEM. We found that changing the ion beam doze and exposure time we can control the nanographite etching depth with the step down to 1 nm. Thus this technique can be used in the nanographite thinning. We also used FIB to graphene nanoribbons of 70 nm width production. The graphene decorated with metal nanoclusters are the basic of self assembling carbon nanostructures development. We investigated the topography and electronic properties of graphene decorated with catalytically active metal particles (Fe, Co, Mn, Cr, Zr and Hg (and/or their oxides). These materials can obtain high catalytic activity defined by their unique structure, high specific surface area and order strength. It was found depending on production temperature varied of 200 to 500 degrees centigrade the nanoclaster size changes from 20 to 500 nm.

## Poster Board | 71

### Highly conductive transparent films with single-walled carbon nanotube using the combination of thermal oxidation and recovery treatment

**Ju Yeon Woo**, *Korea Institute Of Machinery And Materials* | **Hyung Cheoul Shim**, *Korea Institute Of Machinery And Materials; Korea Advanced Institute of Science and Technology* | **Yong Shin Kim**, *Korea Institute Of Machinery And Materials; Korea Advanced Institute of Science and Technology* | **Duck Jong Kim**, *Korea Institute Of Machinery And Materials* | **Joon Dong Kim**, *Korea Institute Of Machinery And Materials* | **Chang Soo Han**, *Korea Institute Of Machinery And Materials*

A simple combination of thermal oxidation and recovery treatment was applied to get the highly purified single-walled carbon nanotubes (SWNTs) films with low sheet resistance. The comprehensive electrical and optical performance, especially the conductivity, could be significantly improved after combination of oxidation and recovery process due to the effective removal of impurities and interconnecting networks of highly wellaligned SWCNT bundles. SWCNT samples were analyzed using Raman spectroscopy, scanning electron microscope (SEM), transmission electron microscope (TEM), and thermo gravimetric analysis (TGA). After efficient procedure of the purification, its sheet resistance decreased from 5000 to 187 Ohm/square with 80% optical transmittance at a wavelength of 550 nm.

## Poster Board | 74

### Mechanism of doping semiconducting carbon nanotube by AuCl3 and their electronic, hygroscopic properties by density functional theory studying

**Dinh Loc Duong**, *Sungkyungkwan University* | **Ilha Lee**, *Sungkyungkwan University* | **Ki Kang Kim**, *Massachusetts Institute of Technology* | **Jing Kong** , *Massachusetts Institute of Technology* | **Seung Mi Lee**, *Korea Research Institute of Standards and Science* | **Young Hee Lee**, *Sungkyungkwan University*

Controlling properties of carbon nanotube by doping is an important step for many applications such as transparent conducting films, nanosensors and thin film transistors. Different doping approaches were proposed. In this work, we investigated the mechanism of doping semiconducting carbon nanotube (s-CNT) by salt solution AuCl3. We propose that s-CNT-Cl complex is a key component in doping CNTs. Although cation Au3+ plays an important role in ionizing s-CNTs as an intermediate precursor, the ionized s-CNTs are neutralized further by forming a stable s-CNT-Cl complex as a final reactant. The electronic and hygroscopic properties of p-type doped s-CNT by AuCl3 were studied. The p-type behavior of s-CNT at the solid state that was caused by the Cl adsorbed on s-CNT surface was confirmed. This localized charged anion site is highly hygroscopic to induce adsorption of water molecule. This opens a new possibility that the anion-functionalized CNTs could be used for humidity sensor as well as dipole molecules.

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### Wave functions and many-body effects in carbon nanotubes measured by STM

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We report here atomically resolved STM/STS investigations of local electronic properties of C-SWNTs. First, we demonstrate the dominant role of many-body interactions in the electronic band gap of carbon nanotubes measured by STS [1]. The novel approach presented here allows us to observe a continuous transition from the screening reduced gap to the intrinsic gap and to determine this latter from STS. Furthermore, comparing STS results with optical absorption measurements on the same sample provides values of exciton binding energies. These results provide a deeper knowledge of many-body interactions in these 1D systems and solve the apparent controversy of the pioneering STM measurements which reported the same gap values than optical experiments [2, 3]. Second,we show for the first time a complete experimental investigation of molecular orbitals of SWNTs using atomically resolved STS [5]. Local conductance measurements show spectacular carbon-carbon bond asymmetry at the Van Hove singularities for both semiconducting and metallic tubes, demonstrating the symmetry breaking of molecular orbitals in nanotubes. Whatever the tube, only two types of complementary orbitals are alternatively observed. An analytical tight-binding model describing the interference patterns of pi orbitals confirmed by ab initio calculations, perfectly reproduces the experimental results [5]. [3] H. Lin et al, Nature Materials, published on line 2010 [2] F. Wang, et al Science 308, 838 (2005). [3] J. W. G. Wildoer et al Nature 391, 59 (1998) ; T. W. Odom, et al, Nature 391, 62 (1998). [4] H. Lin et al arXiv:0911.4437

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### Enhanced spin-valve effect in magnetically doped carbon nanotubes

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Spin valves made of nanotubes contacted to magnetic electrodes may display significant values of magnetoresistance but are limited by the restricted capacity for spin-injection into the tube and by the unwanted spin-flip scattering caused by magnetic impurities. We propose an alternative route to produce the spin-valve effect which (a) does not involve magnetic electrodes, avoiding the spin injection limitation, and (b) uses magnetically coupled impurities to generate an efficient spin filter that enhances the magnetoresistance by orders of magnitude. Furthermore, we predict that substitutional Mn impurities on metallic nanotubes will generate enormously large values of magnetoresistance [1]. [1] D. F. Kirwan, V. M. de Menezes, C. G. Rocha, A. T. Costa, R. B. Muniz, S. B. Fagan and M. S. Ferreira, Carbon 47, 2533 (2009)

## Poster Board | 83

### Defects in carbon nanotubes: heterodoping, structural modifications, and their effects on properties.

**Vincent Meunier**, *Oak Ridge National Laboratory*

The paradox of perfection (i.e. flaws make things perfect) could be the key to designing nanoelectronic circuits from carbon nanostructures, such as nanotubes or graphitic nanoribbons. While individual carbon nanotubes can be exceptionally good conductors, connecting nanotubes into usable circuits is not easy, and in fact the networks realized from the connections between individual nanotubes do not conduct well. In this contribution, I will present an overview of the studies we performed to determine the effects of heterodoping and topological defects on the electronic transport in complex carbon nanostructres. The theoretical findings will be compared to experimental data when available. First, I will present evidence that the transparency of nano junctions can be improved dramatically by adding defects to the connecting ends of the nanonetworks. Second, I will show how these defects can be important for electrochemical energy storage applications. Finally, I will indicate how these findings can be used to devise practical devices with tailored properties.

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### Phase transition in peapods bundles: an ab initio calculation

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The interest in materials at the nanoscale is increasing, mainly due to their potential application in various fields of science and technology. Through improvement of experimental techniques and the development of computers increasingly sophisticated, theoretical and experimental researchers had the opportunity and ability to work together. Nanostructures based on carbon nanotubes have been at the forefront of research of nanomaterials in recent years. Carbon nanotubes (SWCNTs), with its excellent mechanical and physical properties are the prototype of nanoscience in general. In solid form, fullerenes and nanotubes are constituent units of weakly bounded to each other. Currently, interesting forms of carbon have been synthesized, which fullerenes are aligned in a string and encapsulated in carbon nanotubes single wall called Peapods, where refers to kind fullerenes. Accordingly, the electronic structure near the Fermi level are controlled by the inter space between the layers and the distribution of states of almost free electrons. In this work, structural, electronic properties and cohesive energy of C60@ SWCNT subjected to hydrostatic pressure are investigated in order to optimize their physical and chemical properties for potential applications in nanodevices. The calculation is performed using ab initio method based on the theory of density functional implemented in SIESTA computer program. We results indicate that the bundles in the study suffer two phase transition the first transition occurs around at 2.0 GPa and the second transitions occurring approximately a 15.0 GPa.

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### Variations in Hot Phonon Decay Rate Due to Gas Adsorption on Pristine Suspended Carbon Nanotubes

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Optical Raman spectroscopy and electrical measurements are simultaneously carried out on pristine suspended carbon nanotube devices in various gas environments. Devices exhibiting negative differential conductance (NDC) at high bias voltages experience a sudden drop in current (kink) in these gaseous environments. The kink varies in character and magnitude according to the surrounding gas. This kink is attributed to the adsorption/desorption of gas molecules on/off the surface of the nanotube. When the device is electrically biased at the kink, the temperature of the suspended nanotube is determined from changes in the Raman spectra. The temperature measured is found to have the following ordering THe < TAr < TCO2 and is independent of the base substrate temperature. Comparison between measured and simulated I-V characteristics indicates that the desorption of gas molecules changes the decay rate of hot phonons.

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### Optimum geometry for field emission from perfect array of CNTs

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The optimum geometry for field emission from a perfect array of carbon nanotubes (CNTs) has typically been calculated to have a pitch ratio (individual CNT spacing divided by height) of approximately 2. Here, we show that the optimum pitch ratio has a logarithmic dependence on the local electric field, ranging from 7 at low field (1.0 x 105 V cm-1) to 1 at high field (2.5 x 108 V cm-1). These results have been obtained by both numerical modeling and analytical calculations. This relationship occurs due to the exponential dependence of the electrostatic shielding of neighboring CNTs.

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### Spectroscopic Study of the Redox Reactions in Carbon Nanotubes Field-Effect Transistor Operation

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We have identified the oxygen / water redox couple as the responsible for the suppression of electron transport of carbon nanotubes field-effect transistors through a series of controlled gas experiments. [1] We proposed that the Fermi level of the carbon nanotubes is pinned by the chemical potential of the acidic surface water layer resulting from the adsorption of atmospheric gases on the supporting SiO2 gate dielectric. Equilibrium is attained when electrons are transferred from the nanotubes to the surface, where trapped charges are created and screen the electric field applied from the gate electrode, thus impairing the operation of the transistor. The adsorption of a water layer being important for the process, we further investigated the effect of modifying the chemical nature of the substrate. Using hydrophobic substrates ranging from parylene-C to self-assembled monolayers of alkyl silanes, we showed that electron conduction can be obtained in air. Thermodesorption spectroscopy experiments coupled to reflection-absorption infrared spectroscopy under high vacuum conditions were used to probe the surface of transistors. We will discuss the mechanism and the implications of the redox assisted electron transfer in electronic devices made from carbon nanotubes, graphene and organic semiconductors. [1] C. M. Aguirre et al. Advanced Materials, v. 21, p. 3087.

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### Electronic field emission properties of open and capped nitrogen-doped carbon nanotubes

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We used density functional theory calculations to establish the electronic field emission properties of nitrogen doped carbon nanotubes. Our study includes the (5,5), (9,0), and (10,0) nanotubes. All systems were first relaxed using conjugate gradient method. An external electric field was then applied parallel to the tube axis to simulate an electron emission experiment. We calculate the electronic density of states, the binding energy, the energies associated to HOMO and LUMO and the work function for different tip morphologies, tube lengths, and nitrogen concentration. We observed that the symmetry of the nanotube tip and the lenght play a crucial role in the electronic properties. We used our theoretical determination of enhancement factor and work function in conjunction with Fowler-Nordheim expression to make a comparison with experiments.

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### Determination of Redox States of Isolated (n,m)SWNTs in Water

**Yasuhiko Tanaka**, *Department of Applied Chemistry, Kyushu University* | **Naotoshi Nakashima**, *Department of Applied Chemistry, Kyushu University; Japan Science and Technology Agency, Core Resarch of Evolutional Science & Technology (CREST)-CREST*

Ever since the discovery of single-walled carbon nanotubes (SWNTs), many attempts have been made to determine the electronic properties of SWNTs; however, the achieved success in the determination of the oxidation and reduction properties as already reported has been low. Very recently, we have discovered that we can determine the oxidation and reduction potentials of several isolated SWNTs in a film on an electrode by in situ near-IR PL spectroelectrochemistry. Here we report an experimental method for the determination of the oxidation and reduction potentials as well as Fermi levels of (n,m) SWNTs individually dissolved in water based on the Nernst analysis of the in situ PL spectroelectrochemical data of the isolated (n,m)nanotubes.

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### Some aspects of the application carbon nanotubes forest for sensing gases and vapors

**Vyacheslav Khavrus**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Hartmut Vinzelberg**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Joachim Schumann**, *Leibniz Institute For Solid State And Materials Research Dresden* | **Albrecht Leonhardt,** *Leibniz Institute For Solid State And Materials Research Dresden* | **Steffen Oswald**, *Leibniz Institute For Solid State And Materials Research Dresden*

Carbon nanotubes (CNTs) have received much attention due to their high chemical stability and excellent heat conduction. CNTs have a capacious surface and large surface-to-volume ratio. The remarkable sensitivity of CNT conductivity, depending on the surface adsorbates, permits its use for development miniature CNTs-based sensing devices for the detection of various gases and vapors. Available in literature studies of surface properties of different carbonaceous materials have indicated that chemical functionalization of the carbon shells of CNTs would play an important role in tailoring their adsorption properties. However, many intriguing questions remain open. Analysis of published data shows that in the most cases the reproducibility of experiments is quite low and the sensor resistance does not return to the initial value during repetitive measurements at the same conditions or in the inert atmosphere for a long time [1]. To find explanation of this problem, we performed detailed experimental study using dense vertically-aligned “forest-like” CNTs [2]. The aim of the presented work is the investigation of the CNT sensitivity, recovery and selectivity towards different gases at different temperatures. Change in the resistance of the prepared CNTs sensing device in atmosphere of various gases was measured. We discuss the importance of morphology, chemical functionalization and operational history of our CNT device for further development and application of gas sensors. [1] T. Ueda et al. Physica E 40 (2008) 2272–2277 [2] V. O. Khavrus et al. Carbon 45 (2007) 2889–2896.

## Poster Board | 115

### Encapsulation of Single-Stranded DNA inside Double-Walled Carbon Nanotubes

**Yongfeng Li**, *Department of Electronic Engineering, Tohoku University* | **Toshiro Kaneko** | **Hatakeyama Rikizo**

In this work, we present the first investigation of encapsulation and release of single-stranded DNA (ssDNA) molecules inside and from the inner space of double-walled carbon nanotubes (DWNTs) by utilizing DC electric fields of different polarities, respectively, in ssDNA solution. Our results indicate that DNA molecules are easily encapsulated inside large diameter DWNTs, which is confirmed in detail by a transmission electron microscope (TEM) and Raman spectroscopy [1]. The most attractive feature of ssDNA encapsulated DWNTs is that the encapsulated ssDNA molecules are found to be efficiently released from DWNTs by applying an electrical field of the reverse polarity. In addition, it is demonstrated that the electrical transport properties of DWNTs are changed drastically due to the ssDNA encapsulation. Here the charge transfer between the ssDNA bases and nanotubes is shown to highly dependent on the type of the DNA bases, which is possibly explained in terms of their different redox potentials [2]. The unique electronic properties of ssDNA encapsulated DWNTs make them potentially useful in many applications such as molecular electronics, molecule sensor, and gene and drug delivery systems.

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### Optimization procedure of a CNT-based field emission cathode

**Grigory Bocharov**, *Kintech Lab Ltd, Moscow, Russia* | **Alexander Eletskiy**, *Kintech Lab Ltd, Moscow, Russia* | **Timothy Sommerer**, *GE Global Research, Niskayuna, USA*

The optimization procedure of a CNT-based field emission cathode has been elaborated. There has been considered a regular array of vertically aligned nanotubes of equal geometry. The optimization procedure takes into account the field amplification effects, field screening by closely spaced nanotubes and thermal instability limiting the emission current of CNT. The optimization is based on the simultaneous solution of the Laplace equation for the spatial distribution of the electrical field in the vicinity of a nanotube cap, heat conduction equation for a nanotube and Fowler-Nordheim equation interconnecting the electrical field strength at a nanotube tip and the emission current. The optimization procedure results in the optimum inter-tube spacing in the array providing the maximum emission current density. It is shown that the optimum parameters of a CNT array depend on both the applied voltage and aspect ratio of nanotubes comprising the array. The sensitivity of the optimization results to the accepted values of transport parameters of nanotubes (heat conductivity and electro conductivity coefficients) is analyzed.

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### Facile Method to Produce High-Transparency Single-Walled Carbon Nanotube Films and their Thermal and Electrical Properties

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Single-walled carbon nanotube (SWCNT) films are promising candidates for applications requiring transparent conductors due to their low sheet resistance and high transparency in the visible region. Vacuum filtration is a common and easy to implement technique to produce such films but it is complicated by the need to transfer the films to desired substrates. We recently reported conditions under which SWCNT films produced by vacuum filtration detach from the filter membrane upon submersion into water, thereby providing a facile approach to transfer filtration-produced nanotube films to desired substrates [1]. The method, which employs simple laboratory glassware and can be implemented at minimal cost, combines the advantages of vacuum filtration with easy, rapid, solvent-free detachment to obtain high-quality, SWCNT films on transparent substrates. The films were assessed by optical microscopy, UV-vis and Raman spectroscopy, electrical measurements, atomic force microscopy and scanning thermal microscopy. Sheet resistance measurements show that these films are competitive with other high-transparency, conductive SWCNT films made through more cumbersome procedures. The use of nitric acid treatments, either for pre-treating the SWCNTs as in common purification procedures or for post-treating the films, results in superior electrical conductivity in comparison to SWCNT films made with high-purity nanotubes not exposed to acid treatments. Thermal imaging by scanning thermal microscopy indicates that heat dissipation by the film is comparable to that of a glass substrate.
[1] M.B. Jakubinek, M.B. Johnson, M.A. White, J. Guan, B. Simard, J. Nanosci. Nanotechnol. In press (2010).

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### Humidity-assisted selective reactivity between NO2 and SO2 gas on carbon nanotubes

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Adsorption and desorption of $NO_2$ and $SO_2$ gas on carbon nanotubes were investigated in terms of different humidity levels at room temperature. Random network singlewalled carbon nanotubes (SWCNTs) resistor was constructed by a dip pen method using SWCNT/dichloroethane (DCE) solution. The resistance always decreased when $NO_2$ gas was introduced independent of moisture level. On the other hand, the resistance increased with moisture concentration in the case of $SO_2$ gas.This humidity-assisted gas reaction provides a simple way to selectively detect two gases. The change of response time and recovery time with different moisture levels was further studied.

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### Formation of Infrared p-n Junction Solar Cells Based on Single-Walled Carbon Nanotubes

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Single-walled carbon nanotubes (SWNTs) have a good potential for solar cells because of their absorption bands in the infrared light range as well as some advantages such as large surface areas, enormous current carrying capability, high mechanical strength, and chemical stability. In this study, as a crucial step toward the realization of infrared solar cells, electrical properties of p-n junction fabricated using the combination of thin film of SWNTs and n-doped silicon (n-Si) are investigated without or with light illumination. The electrical properties of these SWNT film/n-Si devices show a rectifying characteristic of current-voltage (I-V) curves, and a short-circuit current ISC and an open-circuit voltage VOC through a downward shift of I-V curves are observed under light illumination. In particular, it is found that the device fabricated with the fullerene C60 encapsulated SWNTs (C60@SWNTs) film has a large VOC caused by a large diffusion voltage in the interface of p-n junction compared with the device fabricated with the pristine SWNT film, due to the enhanced p-type behavior of SWNTs after C60 encapsulation. In addition, the electrical properties of p-n junction solar cells based on individual SWNT in which electron donor such as C59N is partially encapsulated have been investigated without or with light illumination.

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### Modulating transport responses on carbon-based Fabry-Perot cavities

**Andrea Latge**, *Universidade Federal Fluminense* | **Monica Pacheco**, *Universidad Tecnica Feerico de Santa Maria* | **Luis Torres**, *Universidad Nacional de Córdoba* | **Claudia Rocha**, *Dresden University of Technology*

Motivated by recent reports on magnetoconductance pattern measured on multi-walled carbon nanotubes under intense pulsed magnetic fields, we propose a theoretical investigation on the conductance spectra of resonant Fabry-Perót cavity composed of carbon nanotubes. The interplay between the effects of homogeneous magnetic fields and time-dependent AC potentials on the tube device is analyzed considering a variety of conjugated potentials. Following the Green formalism and simple tight-binding model calculations we show that the conductance of such electron wave guides exhibit rich Fabry-Perót diagrams. The extra potential imposed by perpendicular magnetic fields induce other changes in the electronic properties of the nanostructured systems allowing also metal-insulator transitions. The transport study indicates that it is possible to select particular AC field intensities and frequencies in order to chose a variety of transport responses, depending on the strength of the magnetic field. Conductance diagrams on Fabry-Perót devices composed of graphene nanoribbons are also discussed.

## Poster Board | 127

### The effect of bundle length and diameter on the performance of SWCNT-network electrodes

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Due to the tendency of nanotubes to bunch together, SWCNT-networks consist of bundles, instead of individual tubes. Several factors, including the contact resistances inside and between bundles affect the electrical performance of the networks. The number of contacts depends strongly on the length and diameter of tubes and bundles. Recent studies have shown that the contact resistance between bundles increases strongly with diameter and that chemical doping has a strong effect on the contact resistance, while the optical absorption level depends mainly on the number of carbon atoms per unit area.  We have studied the effect of bundle diameter and length on the resistance of directly deposited SWCNT-networks. Bundles with average lengths of 1, 3 and 9 µm with corresponding average diameters of 8, 8 and 13 nm were synthesized with a ferrocene based aerosol CVD-process. The bundle length and diameter can be adjusted via synthesis gas additives (CO2) and the reactor temperature. The Hot Wire Generator (HWG) synthesis method can be utilized to fabricate bundles of about 3 µm while offering potential for reduction of the bundle diameter.  The SWCNT-networks can be transferred onto various substrates. When the networks were chemically doped with nitric acid, the sheet resistances at 90% transmittance ranged from 1000 Ohm/square  via 200 Ohm/square to 110 Ohm/square  for the ferrocene synthesized bundles. The HWG-synthesized networks demonstrated also promising performance with 40 Ohm/square sheet resistance at 70% transmittance. The results indicate the importance of controlled bundle diameter and length for high performance SWCNT-network electrodes.

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### KrF laser synthesis of single wall carbon nanotubes and their use for photovoltaic applications

**Vincent Le Borgne**, *Institut National De La Recherche Scientifique* | **Paola Castrucci**, *Tor Vergata University- Department of Physics* | **Maurizio De Crescenzi**, *Tor Vergata University- Department of Physics* | **My Ali El Khakani**, *Institut National De La Recherche Scientifique*

Single wall carbon nanotubes (SWCNTs) were synthesized by ablating a Co/Ni catalyst loaded graphite target with a pulsed KrF excimer laser (248 nm, 20 ns) under appropriate background conditions. The SWCNTs grown at a furnace temperature of °C, are of high quality with a very narrow distribution of diameters centered around 1.2 nm. The obtained SWCNTs were systematically characterized, before and after purification, by means of various techniques, including Raman spectroscopy, electron microscopy and thermogravimetry analysis (TGA).We will report, in particular, on the effect of two main growth parameters, namely catalyst content and furnace temperature, on the nature and structural characteristics of the synthesised carbon nanostructures. While the catalyst content is found to affect directly the nature of the synthesized carbon nanostructures (from fullerene to large diameter SWCNTs), the diameter of the SWCNTs can be reasonably controlled (between 0.8 to 1.4nm) by varying the furnace temperature (from 900 to 1200°C), for the optimal Co/Ni catalyst content of 1.2 at. %. After their purification, our KrF-laser synthesized nanotubes were integrated into planar SWCNTs/Si hybrid photovoltaic (PV) devices and their PV properties assessed. Our results demonstrate the ability of these SWCNTs/Si hybrid PV devices to generate significant photocurrent, of which magnitude can be optimized by SWCNTs film thickness. The results on the quantum efficiency and I-V behaviours of these novel SWCNTs/Si devices will be presented and discussed.

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### Effect of Conductive and Adhesive Fillers on Field Emission Properties of Carbon Nanotube Pastes

**Hansung Lee**, *Sejong University* | **Jeungchoon Goak**, *Sejong University* | **Jusung Choi**, *Sejong University* | **Chungyeol Lee**, *Sejong University* | **Naesung Lee**, *Sejong University*

Recently, carbon nanotube (CNT) emitters looked toward producing high emission currents to provide X-ray dose enough for specific applications. However, many researchers reported the degradation and failure of CNT emitters during extraction of high current emission. We have tried to fabricate X-ray source CNT emitters with high current emission and long-term stability using CNT paste. This study, a major variable of improving the electrical conductivity and adhesion was adopted different approaches to the using two-type fillers of low-melting-point and high-conductivity properties. In our previously study, the composition of the CNT paste varied mainly in the amounts of CNTs and conductive fillers. In particular, the conductive fillers with micro- and nano-sizes were optimized by changing the amounts in the range of 5~15%. Among many combinations of micro- and nano-size conductive fillers, the content of 5% under the mixing ratio of 3:1 produced the best field emission curve. The amount and size of fillers had a considerable effect on the shape, processing stability, and field emission characteristics of CNT emitters. Thus, the addition of a small amount of nano-size fillers seems to be helpful to improve the field emission characteristics of the CNT paste. The effect of added to adhesive filler would also be discussed in detail in comparison to other paste composition.

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### Self-organized networks of carbon nanotubes and their transparent conducting properties

**Suarpa Ketpreechasawat**, *The University of Tokyo* | **Hisashi Sugime**, *The University of Tokyo* | **Yosuke Shiratori**, *The University of Tokyo* | **Suguru Noda**, *The University of Tokyo; PRESTO, Japan Science and Technology Agency*

Single-walled carbon nanotube (SWCNT) networks have emerged as a promising material for diverse thin film electronic devices such as transparent conducting films. Compared with the commonly used metal oxides such as indium tin oxide (ITO), these SWCNT networks offer a higher degree of flexibility and abrasion resistivity as well as their potential for mass production. In this work, SWCNT networks were directly grown on quartz glass substrates to minimize the influence of surfactants. SWCNTs were grown by chemical vapor deposition (CVD) method using either C2H5OH or C2H2 as feedstocks and either Co or Co-Mo as catalysts, and those grown from C2H5OH at ~830 degree C showed good properties. The changes in their morphology resulting from different growth time and catalyst thickness were investigated, and their transparent conducting properties were evaluated. For the growth time shorter than 10 min, films showed high resistivity ~ 10 kohm/sq with high transparency of 90-95%, showing undeveloped SWCNT networks below the percolation threshold. For the longer growth times, films showed moderate resistivities ~ 1 kohm/sq with moderate transparency of 70~90%, showing well-developed SWCNT networks. Interestingly, the transparency-resistivity data of the samples grown by 0.09-1.4 nm thick Co catalysts and 30-60 min were mostly on a single curve, meaning that all these SWCNT networks have similar morphological and thus optoelectrical properties. A post treatment method was examined to densify the networks by exposure to ethanol vapor and a patterned growth was also examined to highly tailor the network morphologies using patterned catalysts.

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### Nanotube polarizability in aqueous medium

**Mariza Grassi**, *GDENB - DFQ - ICE - Universidade Federal De Itajubá* | **Felipe Matuzalem**, *GDENB - DFQ - ICE - Universidade Federal De Itajubá* | **Ana Claudia Carvalho**, *GDENB - DFQ - ICE - Universidade Federal De Itajubá*

Nanotubes have been considered as possible drug delivers and as biosensors. This is mainly due to their unusual physical and chemical properties that allow both selective penetration of biological barriers or functionalization to carry drugs to specific targets, such as cancer tissues. However, the biocompatibility of nanotubes has to be investigated. That makes absolutely necessary to establish the interaction with polar molecules such water, always present at biological materials. The present work presents some results about interaction between water and BN and C nanotubes. Each tube has its geometrical structure previously optimized using MNDO-d semi-empirical method and the interaction was simulated with Molecular Dynamics. Results shows a strong electrical field inside the tube, aligning the water molecules inside the tube and a repulsive field around the external wall, that repels any polar molecule, no matter the chemical composition or chirality of the tube. Also has been noticed the presence of hydrogen bonds between the water molecules inside the tubes and the inner walls .

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### Inkjet-printing of Carbon nanotube network: From dispersion to devices

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Being cost-effective, additive in nature, with no requirement of masks for different device levels, the inkjet printing technology has emerged as a popular and prospective method for fabrication of electronic devices and circuits. The purpose of the present work is to take advantage of this technology to fabricate all inkjet-printed carbon nanotube(CNT)-based electronic devices. Two classes of CNT networks were investigated: Single (SWCNTs) and Multi (MWCNTs) Walled Carbon Nanotubes. Different CNT dispersants along with different types of SWCNTs (HiPCO,CoMoCAT) were used to make dispersions. Transmission Electron Microscopy (TEM) measurements and optical methods were used to characterize CNT morphology and dispersions in respect to the role of different dispersants. After formulation of CNT dispersions, we fabricated all inkjet-printed CNT devices such as CNT field effect Transistors (CNTFETs) and Infra-Red (IR) sensors on flexible Kapton Polyimide. For CNTFETs, we used CoMoCAT SWCNT dispersion as the active region and for the IR sensors, Multi-walled carbon nanotubes (MWCNTs) were used. The printed networks of MWCNTs were investigated as sensitive element for bolometric applications. This application, based on the temperature coefficient of resistance, requires low heat dissipation from the nanotubes to their environment. Instead of using suspended CNT network as observed in the literature, we propose here to print the network on plastic substrate, with the aim to limit the thermalization. We demonstrated that significant photo-signal can be obtained in the infrared range with about -0.07 % change in the resistance of the devices, making the printed devices promising as uncooled infrared sensors.

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### A Kinetic Monte Carlo Model Predicting the Short-Circuit Current of a P3HT-SWNT Planar Heterojunction Solar Cell

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P3HT is often used as the electron donating material in photovoltaic devices. It is generally accepted that the excitons generated in this semiconducting polymer need to diffuse to an interface with an electron accepting material to dissociate so the charges can be extracted out of the device. Examples of electron acceptors are CuPc, C60, PCBM, and more recently SWNTs. Bulk heterojunction (BHJ) solar devices demonstrate today's best efficiencies, but are not as high as previously anticipated. Moreover BHJ devices are difficult to study in a rigorous way due to the degree of uncertainty in the exact device structure. Therefore, we have constructed a kinetic Monte Carlo model that takes into account exciton generation, exciton transport, recombination and dissociation to investigate the photocurrent generation in planar heterojunctions. Including the optical, electronical and structural properties of the different materials, we are able to accurately predict the short-circuit current of a P3HT-SWNT planar solar cell developed in our lab that shows an efficiency of 3%. We are able to expose the mechanism responsible for the previously unexplained maximum current output at a P3HT thickness of 60nm. Generally it is assumed the maximum occurs at a value equal to the diffusion length of excitons in P3HT (8.5nm). The model shows how a combination of bulk exciton dissociation and optical interference effects is responsible for this trend. Based upon the results of this model it will be possible to design solar cells more intelligently and steer them towards higher efficiencies.

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### Spin polarization enhancement in disordered carbon-based systems

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The possibility of using the spin of the electron instead of its charge can lead to a new family of devices. In the so called field of spintronics, the spin of the electron is the ultimate logic bit. In the quest to achieve this goal carbon nanotubes present themselves as possible candidates. In particular, nitrogen-rich carbon nanotubes – the so called CNx nanotubes – could be used as possible binding sites for magnetic impurities that could, in turn, result in spin polarized transport. In this work we show, by means of ab initio electronic transpor calculations, how these nitrogen-rich carbon nanotubes can be used as spintronics devices by incorporating transition metal ions. The resulting structure resembles that of Heme-B molecules which are the active sites in Hemoglobin and thus present in nature. The ions used in the present study, such as iron, cobalt and manganese, present a localized magnetic moment that leads to spin-dependent scattering. Using a combination of density functional theory and non-equilibrium Green's functions, we demonstrate that, in the presence of a large number of magnetic scattering centers the degree of spin polarization of the electronic conductance of initially unpolarized electrons entering the device can reach 100 %. We also show that these devices also present a very large giant-magnetoresistance-type effect when a small mangetic field is applied and the mangetic moments of the impurities is aligned. All these effects are explained in terms of the Anderson localization regime for a long and disordered one-dimensional system.

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### Analysis of the Size Distribution of Single-Walled Carbon Nanotubes Using Optical Absorption Spectroscopy

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The diameter of single-walled carbon nanotubes is an important characteristic to determine their electronic properties and direct further applications in electronics and photonics. However, in all known fabrication methods, the as-synthesized SWNTs are produced in various diameters and chiral angles. A demand currently exists for an accurate and rapid method of evaluating the mean diameter and diameter distribution of bulk SWNTs. In this work[1], the SWNT samples with various diameter distributions are synthesized by the gas-phase CVD approach. A novel method is developed for more efficient evaluation of the mean diameter and diameter distribution of bulk SWNTs from optical absorption spectra. Without making a strict assumption on the form of the diameter distribution, the optical absorption from the transition energies of each nanotube is modelled by summing contributions over the entire absorption spectrum. The transition energies of a SWNT are described by a sum of Gaussian line shapes and known peak positions corresponding to the ETB/MB model (extended tight-binding model including many-body corrections). The highly ill-posed problem is well-resolved by the introduction of a regularization term in the fitting process. Verification of this protocol is based upon statistic analysis of hundreds of high-resolution TEM images as well as comparison with Raman measurements on the same SWNT samples. The very good agreement among different techniques indicates that this approach enables accurate and rapid assessment of diameter distribution and can be extended to bulk SWNTs with various diameter distributions. [1] Y. Tian, H. Jiang, J.v. Pfaler, et al. J.Chem. Phys.Lett 2010, 1, 1143

## Poster Board | 147

### Fluorescent Single-Walled Carbon Nanotubes in Ultra Low Density Silica Aerogels for Optical Sensing Applications

**Juan Duque**, *Los Alamos National Laboratory* | **Gautam Gupta**, *Los Alamos National Laboratory* | **Christopher E. Hamilton**, *Los Alamos National Laboratory* | **Andrew M. Dattelbaum**, *Los Alamos National Laboratory* | **Stephen K. Doorn**, *Los Alamos National Laboratory*

Single-walled carbon nanotubes (SWNTs) have unique mechanical, electronic, and optical properties which make them an ideal material for optoelectronics, nanophotonics, and sensing applications. In order to exploit these unique properties, there is a need to develop a stable solid platform which does not alter these unique properties. Here we report a general route to prepare silica nanocomposite gels doped with individually surfactant stabilized SWNTs suspensions. The gels were obtained by exposing tetramethylorthosilicate (TMOS) vapors to SWNT suspensions. Two surfactant systems, sodium dodecyl sulfate (SDS) and sodium deoxycholoate (DOC), were used to isolate SWNTs. Near-infrared emission from DOC-wrapped SWNTs incorporated into the gels was found to be much brighter than SDS-wrapped nanotubes, but was virtually insensitive to changes in the surrounding environment. In contrast, the photoluminescence signal from SDS-wrapped nanotubes could be quenched by changes in pH, as well as interactions with small aromatic molecules. Subsequent supercritical drying of the DOC-SWNT-TMOS gels resulted in monolithic low-density composites with significant near-infrared emission intensity. These unique solid platforms of fluorescent SWNTs will enable ultrasensitive optical sensors for bio-weapons, gases, and basic research in areas like low temperature excitonic dynamics, exciton-phonon coupling, and energy transfer for photovoltaic applications. , 2, 3, Kimberly A. DeFriend Obrey3, 2, and 1.

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### Optical studies of ultraclean suspended carbon nanotubes with local gates

**Gilles Buchs**, *Kavli Institute Of Nanoscience Delft* | **Gary Steele**, *Kavli Institute Of Nanoscience Delft* | **David Lakatos**, *University of Budapest* | **Maria Barkelid**, *Kavli Institute Of Nanoscience Delft* | **Val Zwiller**, *Kavli Institute Of Nanoscience Delft* | **Leo Kouwenhoven**, *Kavli Institute Of Nanoscience Delft*

The demonstration of optical emission from semiconducting single-walled carbon nanotubes (SWNTs) with direct bandgaps in 2002 has opened a new field for nano-optics. Over the few years since the first report of light emission, important steps such as single nanotube photoluminescence, electroluminescence and photocurrent measurements have been taken. Here we present scanning photocurrent microscopy experiments performed on a new type of devices recently developed in the Quantum Transport group at TU Delft [1,2], where ultraclean suspended SWNTs devices are electrostatically doped by means of local electrical gates. [1] G. A. Steele, G. Gotz and L. P. Kouwenhoven, Nature Nanotech. 4 (2009) [2] G. A. Steele et al., Science 325, 1103 (2009)

## Poster Board | 151

### Study of carbon nanotube serpentines on a crystalline quartz

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A promising material to surpass the fundamental scaling limits is the single-wall carbon nanotubes (SWNTs), which represents the most widely studied form of molecular electronics. Recently, combined surface- and flow-directed growth enables the controlled formation of carbon nanotube serpentines (parallel tube flat segments connected by U-turns) on top of crystalline quartz [1]. In this work we study these carbon nanotube serpentines using Raman spectroscopy. In these serpentines, we have observed the Raman spectra to obtain information about nanotube-substrate interaction. This special sample allows us to analyze this interaction in different tube-substrate relative orientation. The effects on the electronic and vibrational properties of the SWNTs indicate important changes in the properties depending on the tube-substrate orientation and this nanotube-substrate interaction can thus be controlled and measured along the same physical nanotube. These results are clearly related to the tube-substrate interaction resulting from the tube-substrate morphology and formation dynamics, as discussed in our work. [1] N. Geblinger, A. Ismach and E Joselevich, Nature Nanotechnology 3, 195-200 (2008).

## Poster Board | 153

### Excitonic character of high-order optical transitions in individual carbon nanotubes

**Christophe Voisin**, *Ecole Normale Supérieure, Laboratoire Pierre Aigrain, France* | **Stéphane Berciaud**, *Columbia University, USA* | **Hugen Yan**, *Columbia University, USA* | **Bhupesh Chandra**, *Columbia University, USA* | **Robert Caldwell**, *Columbia University, USA* | **Yuyao Shan**, *Columbia University, USA* | **Louis Brus**, *Columbia University, USA* | **James Hone**, *Columbia University, USA* | **Tony Heinz**, *Columbia University, USA*

It is now well established that band-gap optical transitions in semi-conducting nanotubes arise from excitons. However, the question remains unclear for higher optical transitions due to possible coupling to overlapping continua. Furthermore, recent spectroscopic studies pointed out that the measured energies of S33 and S44 transitions seemed inconsistent with the widely accepted scaling laws [1]. Here we examine the character of high-order optical transitions in individual nanotubes of defined structure [2]. Freely suspended single-wall carbon nanotubes are studied by means of combined Rayleigh and Raman scattering, which permits accurate assignment of their chiral indices. We are thus able to perform a careful analysis of the optical resonances at the level of a single and structurally assigned nano-object. Excitons are expected to give rise to Lorentzian absorption profiles whereas free carrier absorption leads to asymmetric profiles related to van Hove singularities in the DOS. The observed Rayleigh profiles perfectly fit to the excitonic model whereas van Hove-like profiles fail to reproduce the data due to a systematic overshoot on the blue side of the line. In addition, a clear phonon side-band is systematically observed 200meV above each resonance of semi-conducting nanotubes. Such a side-band was previously reported for lower transitions and considered an additional evidence for their excitonic nature [3]. Our observations on higher energy transitions clearly support a united excitonic interpretation of optical transitions in semi-conducting nanotubes at least up to the fifth transition. [1] Araujo PRL98, 067401(2007) [2] Berciaud PRB81, 041414(R)(2010) [3] Torrens PRL101, 157401(2008), Plentz PRL95, 247401(2005)

## Poster Board | 155

### Analytical Study of Optical Absorption in Single-Wall Carbon Nanotubes

**Abbas Zarifi**, *Yasouj University*

Optical absorption in carbon nanotubes strongly depends on the polarization direction of the incident light. Optical properties in carbon nanotubes for light polarized parallel to the nanotube axis have been investigated semianalytically however for light polarized perpendicular to the nanotube axis no calculations have been reported so far. We propose a method to be able to obtain the electric dipole matrix in carbon nanotubes for perpendicular polarization and then by virtue of that we investigate the optical properties in carbon nanotubes semianalytically. We focus on the optical absorption spectra of Pi electrons for carbon nanotubes with arbitrary chirality for light polarized perpendicular to the nanotube axis, semianalytically. We get completely different resonant energy positions for different polarization directions. Further some small resonance peaks below and after the two times the nearest neighbor overlap integral all carbon nanotubes show a high resonance peak around that value regardless of their chirality. Semiconducting carbon nanotubes moreover show a very high resonance peak associated to the fundamental gap energy. For metallic carbon nanotubes this peak is less pronounced.

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### Exciton and free carrier electroluminescence from a SWNT observed through simultaneous measurements of electrical conductivity and emission spectra

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Single-walled carbon nanotubes (SWNTs) are expected to be applied to the materials for the small size light emitting devices because of its small diameter and optoelectronic properties. As the origin of electroluminescence (EL) from a SWNT, three different excitation mechanisms: an electron-hole injection injection[1], impact excitation[2], and thermal excitation[3] are reported. However, relationship between electrical conductivity and luminescence has not been clarified. In this study, we investigate the EL mechanism of a SWNT by simultaneous measurements of electrical conductivity and emission spectra. We measured EL spectra from a single SWNT by applying bias and gate voltage. In this experiment, two peaks with the energy of 840meV and 1130meV are observed from a single SWNT, although only one luminescence peak is usually observed from a single SWNT. The results of the simultaneous measurements of the drain current and integrated luminescence intensity as a function of the back gate voltage indicate that the lower energy peak is due to the luminescence by impact excitation and the higher energy peak is due to the luminescence by electron-hole injection injection. The energy difference of the two peaks is ~ 290 meV, which is consistent with the exciton binding energy estimated by the theoretical calculation[4]. These indicate that the lower energy emission is due to the recombination of excitons excited by impact excitation and the higher one is due to the interband recombination excited by electron-hole injection injection.

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### Potential range dependence of impurity-bound exciton states in semiconducting carbon nanotubes

**Yuh Tomio**, *Hokkaido University* | **Hidekatsu Suzuura**, *Hokkaido University*

Impurity-bound excitons and the optical properties in semiconducting carbon nanotubes have been studied within the effective-mass theory and a static screened Hartree-Fock approximation. The impurity scattering induces the mixing between several exciton states consisting of intra- or inter-valley electron-hole pairs and largely modifies these exciton energy levels. In particular, when the potential range of an impurity is much smaller than the lattice constant, the inter-valley electron scattering between the K and K' valleys gets comparable to the intra-valley scattering and thus gives rise to inter-valley mixing of excitons. This leads to the energy splitting between optically active (bright) and inactive (dark) excitons and we find two bound exciton states: a dark bound exciton state with the lowest energy and a bright one with the second lowest energy. The latter causes the exciton peak splitting in absorption spectra. On the other hand, when the potential range is much larger than the lattice constant, we can see that the bound exciton states get degenerate (or disappear) due to the suppression of the inter-valley mixing. With varying the potential range of an impurity, we discuss the properties of the impurity-bound exciton states.

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### Observation of Coherent Lattice Vibrations in Metallic Single-Walled Carbon Nanotubes

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We performed degenerate pump-probe measurements using a femtosecond Ti:Sapphire source on single-walled carbon nanotubes, synthesized by the arc-discharge method (diameter 1.4-1.7 nm) and suspended in aqueous surfactant. Examination of the probe beam transmittance through the sample reveals the presence of strong, photon-energy-dependent, time-domain oscillations which when Fourier-transformed can be assigned to the generation of coherent lattice vibrations of the radial breathing mode and G-mode phonons in metallic carbon nanotubes. This constitutes the first observation of coherent lattice vibrations in metallic nanotubes and these results are compared to previous coherent phonon results on smaller-diameter, semiconducting nanotubes and cw resonant Raman data on same-size metallic nanotubes.

## Poster Board | 165

### Photoluminescence quantum yields of ensemble dispersions of SWNTs in various surfactant solutions

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Photoluminescence has become a key property of semiconducting SWNTs. It is a useful tool for studying solution/dispersion quality, (n,m)-resolved populations of samples, and fundamental properties of these quasi-1D semiconductors. Quantitative analysis is hindered by the lack of knowledge regarding photoluminescence quantum yield (PLQY). Utilising an automated computational approach we have analysed photoluminescence and absorbance spectra for dispersions of SWNTs in numerous common surfactant solutions. We present comparative results for absolute PLQY values in these environments on an (n,m)-specific basis for a number of semiconducting SWNT species. Our work is further informed by AFM and concentration-dependent studies. Published values for PLQYs range across several orders of magnitude, and we find a variation of approach regarding measuring PLQY for ensemble dispersions. We find typical PLQY values for ‘bright’ SWNTs on the order of 0.01, and compare values for different surfactant environments. We propose some standardisation of methodology in this area.

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### Resonant Electronic Raman Scattering in Metallic Carbon Nanotubes

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A new feature in the inelastic light scattering spectrum of metallic carbon nanotubes is reported and attributed to electronic Raman scattering (ERS) from interband electron-hole pairs. The ERS spectrum originates from scattering with a continuum but it is peak shaped because certain excitations are selectively enhanced due to a resonance of the scattered photon with the optical transition energies of the nanotube. Consequently, the spectrum of photons emitted via ERS maps out the transition energies of the metallic nanotube. We discuss the interference between electronic and phonon scattering and relate it to the mild asymmetry that is commonly observed in the lineshape of the G-band Raman feature of metallic nanotubes.

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### Modification of the electronic structure of individual single-walled carbon nanotubes by control of the dielectric environment

**Yang Wu**, *Columbia University, USA* | **Feng Wang**, *University of California, Berkeley, USA* | **Kin Fai Mak**, *Columbia University, USA* | **Jennifer Klare**, *Columbia University, USA* | **Colin Nuckolls**, *Columbia University, USA* | **Tony F. Heinz**, *Columbia University, USA*

We have controllably modified the electronic states of single-walled carbon nanotubes (SWNTs) by depositing pyrene molecules on individual suspended tubes. The induced changes in the band structure were probed using Rayleigh scattering spectroscopy. We show that just a few monolayers of adsorbed pyrene molecules act to red-shift the nanotube excitonic transitions by tens of meV. This behavior is understood as a consequence of dielectric screening of Coulomb interactions by the physisorbed pyrene molecules. The approach allows bandgap engineering along the length of pristine SWNTs by selectively depositing molecules on different segments of the nanotube. We demonstrate here the formation of an 8-micron wide quantum well structure in a semiconducting nanotube. The excitonic potential well depth was found to be 30 meV. Larger shifts in the single-particle band gap are expected.

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### Splitting of the Raman G band in individual and polymer embedded double wall carbon nanotubes

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We observe a clear splitting of the G band for individual double wall carbon nanotubes deposited on a SiO2 substrate due to the inner and outer tube depending on the coupling of the two walls. The coupling of the two walls is influenced by the inter wall spacing. The inter wall spacing varies as a function of the synthesis process and process parameters used such as the growth temperature of the inner and outer tube. We find that agglomeration of tubes into bundles leads to line broadening having the effect that the G band of the inner and outer tubes overlap. Embedding double wall carbon nanotubes in a polymer environment has the effect that the interaction of the outer wall with the surrounding molecules leads to charge transfer and changes in the pressure felt by the tube. This influences the splitting of the G band from the inner and outer tube. When recording Raman images of the G band of polymer composites we use the G band splitting to distinguish between regions where the double wall tubes are well dispersed and interacting with the matrix, and regions where the tubes are agglomerated or bundled. The dispersion of carbon nanotubes in a polymer composite is crucial to guarantee percolation at low tube concentration to evacuate electrical charges or for reinforcement applications. After optimizing the excitation wavelength we can use Raman spectroscopy to detect concentrations of double wall carbon nanotubes as low as 0.8 % in a polymer matrix.

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### Magnetic nanowires confined in narrow DWNT - a promissing material for cancer treatment by hyperthermia

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In this work, performed within the Marie Curie RTN CARBIO (http://www.carbio.eu) dealing with biomedical applications of carbon nanotubes (CNT), we focus on the filling of CNT with magnetic nanowires [1]. Narrow double-walled CNT (DWNT) were prepared by catalytic chemical vapour deposition, using a MgO-based catalyst, which was reduced at 1000°C in a mixture of H2 and CH4, containing 18 mol % of CH4. The selectivity towards DWNT is ca. 80% [2]. Before and after purification in air, these tubes with inner diameters _?_ 2 nm were filled by capillary action with melted iron and cobalt precursors (FeI2, FeCl2, FeCp2 or CoI2), followed by reduction in H2, in order to prepare magnetic nanowires inside the DWNT [3]. The Mössbauer characterizations after reduction of the iron halides@DWNT in H2, have evidenced the presence of

superparamagnetic nanoparticles of Fe(III) oxides (SPION), which present very high interest, as they are sensitive to magnetic fields, without retaining magnetisation after removal of the latter [4].
In parallel, after reduction of the CoI2@DWNT, AGM and SQUID measurements revealed the presence of ferromagnetic nanowires of cobalt confined in DWNT. The samples were further characterized by HRTEM, EDX, TGA and chemical analysis. Hyperthermia measurements were also performed, in order to check the applicability for biomedical tests.   References:  [1] R. Klingeler et al., International Journal of Hyperthermia, (2008), 496 [2] E. Flahaut et al., Chem. Commun., (2003) 1442 [3] C.-M. Tîlmaciu et al., Chem. Commun., (2009), 6664 [4] A.L. Barnes et al., Biomagnetic research and technology, (2007), 5:1

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### Polysaccharide-dispersed SWNTs reinforced alginate hydrogels

**Liangyu Yan**, *Nanyang Technological University* | **Koon Thye Lim,** *Nanyang Technological University* | **M.B. Chan-Park**, *Nanyang Technological University*

Hydrogels are widely used in diverse biomedical applications such as tissue engineering, lubricous coating, implant (e.g. contact lens), and drug and protein delivery due to their high water content, biocompatibility and resemblance to native extracellular matrix (ECM). However, their poor mechanical properties often limit their applications. SWNTs have outstanding mechanical properties and may impart superior mechanical and electrical properties to hydrogels reinforced with them. We have previously already studied O-carboxymethylchitosan (OC), a biocompatible polymer, as dispersants to finely disperse SWNTs in aqueous solutions. OC can disperse SWNTs well so that the nanotubes exist in solutions as individual tubes or small bundles. OC noncovalently wrapped around SWNTs without damaging their structures. Different ratios of SWNTs well dispersed with OC were added into the alginate hydrogels. Hydrogels reinforced with 1 weight percent SWNTs show compressive properties (i.e. modulus and strength) which increased as much as two times that of unreinforced alginate hydrogel controls. Compared to sodium dodecyl sulfate (SDS) as dispersant, OC demonstrated much higher reinforcing enhancement than SDS. For electrical properties, hydrogels reinforced with 0.5 wt% SWNTs dispersed by OC have lower impedance and higher charge capacity compared with unreinforced alginate/OC hydrogel. These results show that SWNTs can improve the mechanical and electrical properties of alginate hydrogels.

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### Investigation of the Effect of Carbon Nanotube on Electroporation

**Mehdi Shahini**, *University of Waterloo* | **John T.W. Yeow**, *University of Waterloo*

A variety of methods have been employed for cell lysis. Electrical cell lysis, namely electroporation, has several advantages. In these systems, no chemical is necessarily added to the sample cells. And, electrical cell lysis methods are potentially straightforward to be implemented into microelectromechanical systems. However, the high voltage requirements oppose cell lysis to be achieved in lab-on-a-chip technology. Some techniques have been developed to ease this limitation. For instance, the microfluidic device can be designed in such a way that the electric field is locally strengthened in very small areas of interest. Nevertheless, those flow-through microchannels are very likely to be blocked. Moreover, due to uniquely high aspect ratio of CNTs, they are incorporated to produce concentrated electric field locally at the tip of CNT, based on the physics of lightning rod effect. It is reported that the presence of CNT grown on one electrode enhances cell lysis to occur at lower voltages. However, the optimum alignment of CNT on electrode has not been studied yet. At the present work, we have fabricated a 50-micrometer channel, where the E. coli cells are lysed while passing through electrodes. One ITO-coated electrode is on the top and the other electrode made of stainless steel is at the bottom of the microchannel on which the CNTs are deposited. The results show that with the presence of CNT, the required voltage for 100% cell lysis rate is reduced to half. Furthermore, the effects of randomly and vertically aligned CNT on cell lysis are investigated.

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### Thermogravimetric analysis of NIST's single-wall carbon nanotube reference material

**Elisabeth Mansfield**, *Nist* | **Stephanie Hooker**, *Nist*

Single-walled carbon nanotubes (SWNTs) are a promising nanomaterial with applications to aerospace, electronics and biotechnology. However, the properties of different batches of carbon nanotubes can vary considerably depending on chemical purity and the nanotube types present (e.g. diameter and chirality distribution). The National Institute of Standards and Technology (NIST) has developed a single-wall carbon nanotube reference material to allow carbon nanotube manufacturers to have a well-characterized material. Thermogravimetric analysis (TGA) provides one measure of nanotube purity by assessing the material's thermal stability (i.e. how it oxidizes with temperature) by monitoring weight loss as a function of temperature. Results of the raw soot, evaluated for composition with TGA will be presented. Length-sorted fractions of the SWCNT reference material (long, medium, short) will also be available and TGA characterization of each of these fractions will be demonstrated.

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### High resolution electron energy loss and optical absorbance spectroscopic studies of pristine SWCNTs produced by HiPCO process for bio-application

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Single-walled carbon nanotubes have been synthesized by a gas-phase CO decomposition (HiPCO) process, involving high-pressure disproportionation of CO as carbon feedstock and catalytic iron particles were obtained from pyrolysis of Fe(CO)5. The diameter and diameter distribution of as grown material dependents on various parameters, the strong is the pressure of CO cold transverse the Fe(CO)5, nozzle geometry and position for the injection of the reactant in the reaction chamber to produce smaller diameter (about 0.9 nm) at higher CO pressure. The HiPCO materials containing iron were purified by a two-step process of oxidation in oxygen atmosphere and successive washing the mixture of hydrochloric and nitric acids neutralised and distilled water (1:1:1). The optical and electronic properties of the pristine and purified SWCNTs were studied using optical absorption and infrared and Raman spectroscopy. In addition, high-resolution electron energy-loss spectroscopy in transmission was used to analyse the loss and dielectric functions, electron diffraction and core level excitations. The degree of purification and optimisation of the synthesis parameters achieved was estimated using high resolution transmission electron microscopy. Furthermore, the present procedure has a no sufficiently change in the diameter and diameter distribution after Gaussian fit of the optical absorbance spectra. The estimation of the degree of purification is possible by the analysis of core level excitation; finally high purity SWCNTs were obtained for bio-application.

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### Comparative ecotoxicological study in water of double and multi walled carbon nanotubes

**Périne Landois**, *CEA-Saclay Laboratoire Francis Perrin; Institut Carnot Cirimat,France* | **Florence Mouchet**, *EcoLab (Laboratoire d'écologie fonctionnelle), France* | **Pascal Puech**, *CEMES, France* | **Laury Gauthier**, *EcoLab (Laboratoire d'écologie fonctionnelle), France* | **Emmanuel Flahaut**, *Institut Carnot Cirimat,France*

The increased production of carbon nanotubes (CNT) raises questions about their potential effect on health and environment and therefore justifies the need for studies in this direction. A comparative study of the effect of CNT on amphibian larvae in aquatic media (ultimate receptacle of all pollution) will be presented. The potential impact of carbon nanotubes was investigated under normalised laboratory conditions according to the International Standard micronucleus assay (ISO 21427-1) for 12 days of half-static exposure in water. Three different endpoints were carried out for 12 days of exposure: mortality, growth inhibition, and micronuclei induction in erythrocytes in the circulating blood of larvae. Raman spectroscopy analysis was used to investigate the presence of CNT in the biological samples. Considering the high diversity of CNT according to their different characteristics, multi-walled carbon nanotubes were analyzed in Xenopus larvae, comparatively to double-walled carbon nanotubes in similar conditions. Growth inhibition in larvae exposed to CNT was also evidenced, and no genetoxicity (micronucleus assay) was noticed, whatever the concentration as in the case of DWNT. CNT localisation in the larvae leads to different possible hypothesis of mechanisms explaining toxicity in Xenopus. These results will be presented and discussed insisting on the difficulties of current assays of ecotoxicity of carbon nanotubes.

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### Analogies of particle networks in CNT and CB filled epoxy: Assessment through rheological and electrical analysis

**Jan Sumfleth**, *Technische Universität Hamburg-Harburg* | **Carolin Schulz**, *Technische Universität Hamburg-Harburg* | **Wolfgang Bauhofer**, *Technische Universität Hamburg-Harburg* | **Karl Schulte**, *Technische Universität Hamburg-Harburg*

The formation and transition of carbon nanotube (CNT) and carbon black (CB) networks is assessed by means of rheological and electrical measurements. The nanoparticle filled epoxy suspensions as well as the cured nanocomposites exhibit percolation phenomena in rheological and electrical properties at subsequently different percolation thresholds due to dynamic reagglomeration effects taken place in the suspensions. Comparing CB and CNT filled systems, the CNT systems offer improved electrical properties. Mixtures of CB and CNTs in epoxy exhibit an almost identical signature as the CNT epoxy systems, referred to synergistic effects. Independent on the type of nanoparticle, the difference in percolation thresholds is up to one order of magnitude, reflecting strong reagglomeration dynamics. The shear rate dependent formation of particle networks in epoxy suspensions is simulated by means of transient shear experiments with in situ conductivity and optical microscopy analysis. Above rheological percolation, the epoxy suspensions exhibit shear thinning flow behaviour leading to a subsequent decrease in apparent viscosity and conductivity with increasing shear rate. Conversely, at or below rheological percolation, the mechanical agitation leads to increasing viscosities and conductivities. After test times of 75 min, the suspensions reach constant properties reflecting an equilibrium state of dispersion. Here, CB and CNT suspensions exhibit identical viscosities and conductivities giving rise to strong similarities in network morphologies and their formation due to cluster aggregation. In conducting hysteresis tests the network changes were found to be non-reversible, emphasising the need for understanding network forming processes during manufacturing of nanocomposites or fibre reinforced nanocomposites.

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### Multifunctional single-walled carbon nanotube–cellulose composite paper

**Robin Anderson**, *National Research Council Canada-SIMS* | **Jingwen Guan**, *National Research Council Canada-SIMS* | **Michelle Richard**, *FP Innovations - Paprican Division* | **Girjesh Dubey**, *National Research Council Canada-SIMS* | **Benoit Simard**, *National Research Council Canada-SIMS*

Single-walled carbon nanotubes (SWCNTs) have been used as fillers to produce electrically conductive composite papers.(1) While conductive composite papers have been made using other fillers, they either suffer from instability or low conductivity. Using simple papermaking techniques, we have made SWCNT–cellulose composite paper which possesses a conductivity of 300 S/cm and is comparable to or exceeds other reports of carbon nanotube–cellulose papers made by layer-by-layer assembly. These composite papers are multifunctional, having both improved electrical conductivity and enhanced flame retardant properties over the control paper. (1) R. E. Anderson, J. Guan, M. Ricard, G. Dubey, J. Su, G. Lopinski, G. Dorris, O. Bourne, B. Simard J. Mater. Chem., 2010, DOI: 10.1039/b924260k

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### Preparation and Characterization of Transparent, Conductive and Electrochromic Thin Films of Carbon Nanotubes/Prussian Blue Nanocomposites

**Edson Nossol**, *Federal University Of Parana, Brazil* | **Aldo Jose Gorgatti Zarbin**, *Federal University Of Parana, Brazil*

Nanocomposite materials formed by the combination of Prussian Blue (PB) and carbon nanotubes (CNTs) present several interesting properties. PB has a general formula FeIII4[FeII(CN)6]3.nH2O and presents important redox, ferromagnetic and multi-electrochromic properties. We recently developed an innovative route to prepare a CNT/PB composite paste electrode (with high sensitivity to H2O2 detection), based on an in situ electrochemical reaction between the iron-based compounds present in the cavities of carbon nanotubes and the ferricyanide ions in solution [1]. Here we demonstrate that this route can be extended to other kind of electrodes, and show by the first time the electrochemical preparation of thin and transparent CNT/PB electrodes, starting from a transparent film of Fe-filled CNTs. The CNT films were prepared by drop-drying and show good homogeneity and a transmittance at 550 nm varying from 81 to 87%. After the electrochemical reaction with the ferricyanide ions, the gray-black films became blue, and the transparence at 550 nm varies from 58% to 80%. The films present the electrochromism characteristics of the PB (white to pale green to blue), and excellent electrochemical stability, witch makes them promising candidates to be used in electrochromic devices. The PB was characterized by cyclic voltammetry, UV-Vis spectroscopy, XRD, SEM and Raman spectroscopy. A strong interaction between the PB and the CNTs, resulting in a p-doping on the carbon nanotubes, was also detected through these techniques. Acknowledgments: Brazilian Network on Carbon Nanotube Research, INCT-Nanocarbono, CNPq, CAPES-PROCAD. [1] NOSSOL, E., ZARBIN, A. J. G., Advanced Functional Materials, v.19, p.3980, 2009.

## Poster Board | 206

### Synthesis of metal oxide-filled MWNT for insensitive energetic nanomaterials

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Nanothermites are useful energetic nanomaterials for pyrotechnic igniters, actuators, microthrusters and other applications. They are composed of a metal oxide (oxidizer) and a reducing metal (fuel) such as aluminum. As safety has become one of the main criteria for selecting energetic materials for industrial use, the search for insensitive energetic materials is crucial. Our concept for reducing this sensitivity is the physical separation of oxidizer and fuel by enclosing the former into carbon nanotubes, thus reducing the contact area between the two phases. This concept has been proven for the manganese oxide/aluminium system in an earlier communication (B. Siegert, M. Comet, O. Muller, Y. Suma, D. Spitzer, Synthesis of an MWNT/manganese oxide nanocomposite for use in insensitive nanothermite mixtures, in: NT09, Beijing, China, 2009). Here we present the extension of this concept to other metal oxides: multi-walled carbon nanotubes (MWNT) were manganese, chromium, vanadium and copper oxide. Two synthesis methods were used: (a) infiltration of a precursor solution into oxidized (opened) MWNT and (b) a “reactive infiltration” technique combining opening and filling in one step. The products are characterized by X-ray diffraction, TEM, thermal analysis (TG/DSC), Raman spectroscopy and nitrogen adsorption (BET). Nanothermites are prepared by physical mixing of the filled nanotubes with aluminum nanoparticles. Their burning behavior and the activation energies are measured by Time-Resolved Cinematography by igniting pellets by a CO2 laser. We find a reduction in the friction sensitivity of several orders of magnitude compared to a reference nanothermite mixture, leading to a greatly improved operational safety.

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### Composite of aligned CNT/SiC foam with macroscopic shaping for Fischer-Tropsch synthesis reaction

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One-dimensional carbon nanotubes material with high aspect ratio and good thermal conductivity, have witnessed an overincreasing scientific interest especially in the field of heterogeneous catalysis. However, in the bulk form, they present hazardous handling to respiratory system and detrimental pressure drop along the catalysts bed, especially for the fixed-bed catalytic reaction. We were interested to develop an easy handle carbon nanostructure with macroscopic shaping by immobilization them on the macroscopic support. Our work is focused on the synthesis of aligned carbon nanotubes (A-CNTs) on silicon carbide foam structure with a controlled macroscopic shape and its subsequence use as catalyst support for the demanded Fischer-Tropsch synthesis reaction. A-CNTs were deposited on the SiC surface by Chemical Vapor Deposition (CVD) method using ferrocene as a iron-precursor catalyst and toluene as a carbon source. Such prepared A-CNT/SiC composite presents good thermal conductivity, high surface-to-volume ratio which greatly facilited mass and heat transfer and negligible pressure drop. This composite support was further impregnated with cobalt active phase and tested in the exothermic Fischer-Tropsch synthesis. The catalytic performance, i.e. activity and liquid hydrocarbons selectivity, obtained on this catalyst is the highest ones amongst the different state-of-the-art catalysts for the studied reaction.

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### Use of Plasmafunctionalised MWCNT Bucky Papers in Melt-mixed Composites with Polycarbonate

**Petra Pötschke**, *Leibniz Institute of Polymer Research Dresden, Germany* | **Uwe Vohrer**, *Fraunhofer Institute Interfacial Engineering and Biotechnology, Germany* | **Nicolas Zschoerper**, *Fraunhofer Institute Interfacial Engineering and Biotechnology, Germany; University of Stuttgart, Institute for Interfacial Engineering, Stuttgart, Germany* | **Björn MOLLER**, *Fraunhofer Institute Interfacial Engineering and Biotechnology, Germany; University of Stuttgart, Institute for Interfacial Engineering, Stuttgart, Germany*

Multiwalled carbon nanotubes (MWNT) in the form of bucky papers were modified using an Ar/O2 plasma. The effect of plasma modification on the nanotubes was followed by XPS indicating the formation of carboxylic or ester groups at the nanotubes’ surfaces. Nonmodified and modified nanotube materials were incorporated into polycarbonate by melt mixing using a small scale microcompounder. The nanocomposites containing plasma modified nanotubes featured better macrodispersion as characterized by light microscopy than those prepared using nonmodified bucky papers. The electrical percolation threshold was found below 0.5 wt.% which is comparatively low. Mechanical properties in tensile test are slightly affected in terms of enhanced stress values at yield point, higher stress values beyound the yield point and higher stress at break in comparison to nanocomposites with nomodified tubes. The effects can be explained by a combination of better phase adhesion between the modified MWNT and the polycarbonate and better dispersion of the nanotubes. Enhanced adhesion could be also observed using SEM analysis of cryofractured surfaces. The results indicate that the surface modification of multiwalled carbon nanotubes as obtained by simple Ar/O2 plasma treatment without further reactions can induce changes in the composite properties even when melt mixing at high temperatures and relatively short mixing times is applied as the method of composite preparation. This shows the high potential of such a simple nanotube treatment for industrial applications using melt processing as mixing or shaping technique. P. Pötschke, U. Vohrer, N. P. Zschoerper, B. P. Moller, Macromol. Rapid Commun 2009, 30, 1828.

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### Effect of AC and DC electric field alignment of carbon nanotubes modified epoxy composites

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The high electrical conductivity of carbon nanotubes (CNT) has created considerable interest in CNT-based polymer composites for applications requiring electrical characteristics such as electrostatic charge dissipation and electromagnetic interference shielding [1]. Alignment of CNT has previously been reported to increase the conductivity of CNT nanocomposites [2]. This work presents a simple method to control and monitor the alignment of single-walled carbon nanotube (SWCNT) modified epoxy thin films by applying AC or DC voltage. Unfunctionalized SWCNT were produced through a laser technique and dispersed into a high temperature aerospace grade epoxy (MY 0510 Araldite) in an amount slightly above the percolation threshold. During curing of the composite, the current-time curves showed that an AC voltage field produces a maximum current followed by a plateau at 90% of the peak value. This suggests that optimal conductivity occurs in a partially aligned network. For DC alignment, the current-time curves rapidly reached a maximum current followed by a sharp drop (1-2 orders of magnitude). This suggests the formation of an initial aligned network, followed by migration of the polarized SWCNT. Conductivity measurements of the cured thin films show an increase of two orders of magnitude from the isotropic control sample (8x10-7 S/cm) to the AC aligned sample (8x10-5 S/cm) while the DC sample shows a slight improvement over the isotropic material (3x10-6 S/cm). [1] R. Ramasubramaniam et. al., Applied Physics Letters, 83, 2928 (2003). [2] F. Du et al., Physical Review B, 72, 121404-1 (2005).

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### Reactive Spinning of Epoxy Composite Fibers Reinforced with Single-Walled Carbon Nanotubes Grafted with Dendritic Poly(amidoamine)

**Wei Yuan**, *Nanyang Technological University* | **Jianfei Che**, *Nanyang Technological University* | **Mary Chan-Park**, *Nanyang Technological University*

Homogeneous dispersion of single-walled carbon nanotubes (SWNTs), strong SWNT/polymer interfacial strength and good SWNT alignment remain as challenges in exploiting excellent mechanical properties of SWNTs in high-performance structural composites. Covalent functionalization of SWNTs is an effective option in enhancement of composites. We have functionalized SWNTs by grafting with generation (n) 0 to 2 dendritic poly(amidoamine)

(PAMAM) (denoted as SWNT-Gn-NH2, n = 0, 1 or 2) via “grafting from” method. Fourier Transform Infrared (FTIR), hydrogen nuclear magnetic resonance (1H-NMR) spectroscopy and thermogravimetric analysis (TGA) confirmed the successful grafting of PAMAM. Epoxy composite fibers reinforced with PAMAM-functionalized SWNTs were produced by first dispersing the SWNTs in epoxy via solvent blending, followed by pre-polymerization, spinning and then multiple-stage curing. The good nanotube dispersion, strong nanotube/epoxy adhesion and nanotube alignment along the fiber axis were evidenced by field-emission scanning electron microscopy (FE-SEM). The composite fibers reinforced with SWNTs-G2-NH2 show high tensile strength and Young’s moduli per unit weight fraction (dE/dWNT and dE/dWNT) of 3666 MPa and 106.0 GPa respectively, indicating high enhancement efficacy.

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### Chemical and Light Sensors Based on Functionalized Single Walled Carbon Nanobud Networks

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Recently, different types of CNT-based sensors have attracted tremendous attention. They can be made sensitive, ultra compact and with low power consumption. Additionally low fabrication cost can be reached when usages of CNT networks [1]. However, CNT based sensors have low selectivity. Typically, CNTs must be functionalized. Functionalization of CNTs is a challenge due to their chemical inertness. Carbon nanobud (CNB) is a novel nanoscale hybrid material consisting of fullerenes, covalently attached to the outer surface of CNT [2]. CNBs have much higher chemical reactivity in comparison to CNTs and allow the charge transfer between fullerenes and nanotubes. These properties make CNBs promising sensor material. In this work we present experimental results of a systematic study of light and gas sensors based on functionalized CNB networks. Tetrapyrydilporphyrine was utilized as a photo active dye and Nile Blue was chosen as an alcohol sensing molecule. Bingel reaction or a mild oxidation treatment was used for chemical attachment of sensing molecules to the CNB surface. Two principles are used in sensors: measurement of film resistivity and drain current of field-effect transistors (FET) built on functionalized CNB networks. Reversible changes in resistivity and FET drain current are found when the devices are exposed to light or alcohol vapor. The ethanol sensors have a sensitivity with linear dependence on ethanol concentration (~0.8 dR/R, % on mol.%) and minute scale response rate.  1. Zavodchikova M.Y., et al.// Nanotechnology, 2009, V. 20, 8, p.85201 2. Nasibulin A.G., et al.// Nature Nanotechnology, 2007, V. 2, 3, p.156

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### What kind of 3D hierarchical architecture can be formed based on 1D carbon nanotubes and 2D flakes?

**Qiang Zhang**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology* | **Meng-Qiang Zhao**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology* | **Jia-Qi Huang**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology* | **Fei Wei**, *Beijing Key Laboratory Of Green Chemical Reaction Engineering And Technology*

Combining materials with 1D nanowires/nanotubes and 2D lamellar flakes leads to 3D hierarchical nanocomposites with unexpected properties for unique applications. In this contribution, we reported our recent progresses on the directed synthesis of a family of hierarchical architectures with CNTs and lamellar flakes by simple CVD. If we distrusted a high density of catalyst particles on both sides of a flake, levorotatory or dextrorotatory CNT arrays were in situ twisted into a double helix can on a single calcined layered double hydroxide flake [1]. When the catalyst density decreased, a hierarchical composites of single-/double-walled CNTs interlinked with flakes were constructed [2]. What¡¯s more, if the flakes were exfoliated during CVD growth of CNTs, a hybrid composite by intercalating vertically aligned CNTs into layered natural compounds was obtained [3]. Other kinds of 3D hierarchical architecture, such as radial growth of super long CNTs, aligned CNT parallel to flakes, flakes dispersed into aligned CNTs, hybrid of alternating graphene/CNTs, will be fabricated. The present reported strategies provide a quite easy way to provide large amount of samples for the application exploration [4].  Reference: [1] Zhang Q, et al. Angewandte Chemie International Edition. 2010, doi: 10.1002/anie.200907130. [2] Zhao MQ, et al. Advanced Functional Materials 2010, 20(4):677-685. [3] Zhang Q, et al.. Advanced Materials 2009, 21(28):2876-2880. [4] Zhang Q, et al. Carbon 2010, 48(4):1196-1209.

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### Carbonization of polybenzimidazole-wrapped carbon nanotubes and their oxygen reduction activity

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Polymer electrolyte fuel cell (PEFC) electrocatalyst at a cathode electrode is generally composed from catalyst (Pt), electrolyte and carbon support. However PEFC using non-precious metal as a catalyst are the strong request from industry side because Pt is exhaustible asset. One of the promising approaches for the non-precious metal cathode catalyst is the nitrogen-containing graphite structure proposed by Ozaki et al., which were prepared from pyrolysis of the metal complex of nitrogen-containing polymers. We recently reported the pyridine-containing polybenzimidazole (PyPBI) adsorbed to multi-walled carbon nanotubes (MWNT) surface through $\pi$–$\pi$ interaction and act as the solubilizer. By using the MWNT/PyPBI composite thus obtained, we fabricated the cobalt(II) complex of the MWNT/PyPBI (MWNT/PyPBI/Co) and the composite was subjected to carbonization at 600°C for 1 h. The pyrolyzed MWNT/PyPBI/Co was washed with concentrated HCl in order to remove the cobalt species. N1s spectrum of X-ray photoelectron spectroscopy for pyrolyzed MWNT/PyPBI/Co complex showed the change of N-bond states by carbonization. Catalytic activity of the pyrolyzied MWNT/PyPBI/Co complex was monitored by rotating electrode voltammetry in 0.5 M H2SO4 as an electrolyte. It is obvious from the comparison of the voltammograms under nitrogen flow with oxygen flow, the composite sample exhibited oxygen reduction activity.

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### Size-homogeneous metal nanoparticles decorated on multi-walled carbon nanotubes via MeV electron beam irradiation

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The extraordinary properties of carbon nanotubes (CNTs) associated with one-dimensional structure make them into fascinating material having a high potential in various application fields. In particular, a decoration of carbon nanotubes with metal nanoparticles (NPs) is of great interest for applications of hydrogen storage, gas sensor, catalysts for chemical reaction, CNT-based magnetic composites, low-resistance Ohmic contact CNT-based electronic devices. There have been various approaches to obtain the decoration of CNTs with metal NPs, such as a thermal evaporation, electrodeposition, and wet chemical route. Since the properties of the metal nanoparticles can be influenced by their size, it is a crucial issue to obtain the size-homogeneous metal nanoparticles. Here, we report an ingenious strategy, irradiation of MeV electron beam (e-beam) at room temperature under ambient condition, for obtaining size-homogeneous Ni and Pt nanoparticles (NPs) decorated on multi-walled carbon nanotubes (MWNTs). The nano-particlization promoted by MeV e-beam irradiation was investigated by transmission electron microscopy, electron energy loss spectroscopy elemental mapping, and energy dispersive X-ray spectroscopy. These results clearly revealed that Ni and Pt NPs with 5.16 +/- 0.74 nm and 1.63 +/- 0.15 nm in mean size were decorated along the surface of the MWNTs after 2 MeV-e-beam irradiation. A chemical transformation and charge transfer for the metal NPs was systematically explored by X-ray photoelectron spectroscopy and Raman spectroscopy.

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### One Step Mechanosynthesis of Carbon Nanotube Polyaniline Nanocomposites

**Juan Carlos Garcia Gallegos**, *Instituto Potosino De Investigacion Cientifica Y Tecnologica* | **Yadira Itzel Vega Cantu**, *Instituto Potosino De Investigacion Cientifica Y Tecnologica* | **Fernando Jaime Rodriguez Macias**, *Instituto Potosino De Investigacion Cientifica Y Tecnologica*

A new one step mechanosynthesis of carbon nanotube polyaniline (PAni) nanocomposites has been developed. This process was carried out using an organic solvents and acids free method. These nanocomposites were synthesized by ball-milling aniline hydrochloride, iron chloride, multi-wall carbon nanotubes doped with nitrogen (CNx), multi-wall carbon nanotubes (MWNT) and distilled water. Nanocomposites of PAni/MWNT, PAni/CNx and PAni/MWNT/CNx were obtained. The optimum conditions for PAni yield and electrical conductivity of nanocomposites were found by a surface response experimental design measuring the effect of several factors as volume of distilled water, milling time, quantities of MWNT and CNx and the [iron chloride]:[aniline] molar ratio. For maximum PAni yield, a relatively high levels of water volume and [iron chloride]:[aniline] molar ratio was necessary, and it was found that the electrical conductivity was required was determinated mainly by the amount of MWNT. A relatively short milling time was sufficient to obtain these nanocomposites. Their morphology was analyzed by means of SEM/STEM microscopy that indicated a good dispersion of undamaged carbon nanotubes in nanocomposites. Their structure, cristallinity and electrical conductivity were obtained by Raman Spectroscopy, XRD, and Four Points Method, respectively.

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### From Two- to Three- dimensional carbon nanotube networks transparent films: preparation and electrical conductivity

**Mônica Jung de Andrade**, *Federal University of Rio Grande do Sul* | **Marcio Dias Lima**, *University of Texas at Dallas* | **Carlos Pérez Bergmann**, *Federal University of Rio Grande do Sul*

Ultra-thin, optically transparent and electrically conducting films of pure carbon nanotubes (CNTs) and their composites are widely studied thanks to their promise for broad applications. In the present work, we prepare and compare the electrical conductivity of two- and three- dimensional carbon nanotube networks. To produce two-dimensional CNTNs, single-walled CNTs (SWCNTs) were deposited over amorphous silica substrate through the following techniques: dip-coating and electrophoretic deposition. To produce three-dimensional CNTNs, SWCNTs-SiO2 films were prepared by an inorganic sol-gel route and using dip-coating method to deposit over amorphous silica substrate. Both 2D and 3D CNTNs were characterized by atomic force microscopy (AFM), Raman and UV-vis spectroscopies, while their electrical conductivities were evaluated by 4-probe method. In terms of 2D CNTNs, dip-coating and electrophoretic deposition provided quite smooth CNTNs and have great potential for solar cell applications. The obtained characteristics surface resistance and transparency in the UV (550 nm) also demonstrated possible applications in displays, touch screens, shielding in cathode tubes and electrostatic dissipation. In terms of 3D CNTNs, a decrease in the electrical conductivity in comparison to 2D CNTNs was observed, as expected (contact resistances between matrix and SWCNTs).

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### Growth of Single-Walled Carbon Nanotube Carpets from Alumina-Supported Fe Catalysts: Role of Alumina Type

**Placidus Amama**, *Wright-Patterson Air Force Research Laboratory, AFB; UDRI, University of Dayton* | **Cary Pint**, *Smalley Institute for Nanoscale Science and Technology, Rice University* | **Seung Min Kim**, *Birck Nanotechnology Center, Purdue University* | **Kurt Eyink**, *Wright-Patterson Air Force Research Laboratory, AFB* | **Eric Stach**, *Birck Nanotechnology Center, Purdue University* | **Robert Hauge**, *Smalley Institute for Nanoscale Science and Technology, Rice University* | **Benji Maruyama**, *Wright-Patterson Air Force Research Laboratory, AFB*

The important role alumina plays as a catalyst support in single-walled carbon nanotube (SWNT) carpet growth is unsurprising as it is a well known structural modifier or catalyst promoter in hydrocarbon reforming and ammonia synthesis reactions. Although a lot of studies have been carried out so far to explain the role of alumina and the Fe-alumina interaction in the these reactions, an important area of SWNT growth that has not yet been studied explicitly is how the type of alumina affects the activity and lifetime of the catalyst, and the growth termination process. Here, we explore the Ostwald ripening behavior, catalyst lifetime, and mass loss (or sub-surface diffusion) of Fe catalysts deposited on different alumina supports: (a) sapphire; 10 nm thick alumina film deposited by (b) atomic layer deposition (ALD), (c) e-beam, (d) annealed e-beam, and (e) magnetron sputtering. The study reveals a strong dependence of the Ostwald ripening behavior, SWNT carpet height or the catalyst lifetime on the type of alumina used as catalyst support. TEM, ellipsometry, and XPS have been used to account for the marked differences observed.

## Poster Board | 266

### Synthesis of very long multiwall carbon nanotube bundles and their application into polymer-carbon nanotube composites

**Young Chul Choi**, *R&D Center, Hanwha Nanotech* | **Jun Seop Kim**, *R&D Center, Hanwha Nanotech* | **Sang Kyu Choi**, *R&D Center, Hanwha Nanotech* | **Kwang Seok Jeong**, *R&D Center, Hanwha Nanotech* | **Shin Je Cho**, *R&D Center, Hanwha Nanotech*

We have synthesized very long (~500 micrometer) multiwall carbon nanotube (MWCNT) bundles by chemical vapor deposition, and then characterized their structural and electrical properties. The novel catalyst was prepared and its role for the production of MWCNT bundles was investigated. Scanning electron microscopy revealed that the MWCNTs were synthesized as either bundled (aligned) or entangled structures depending on the catalyst system. The yield and the nature of the MWCNT bundles were greatly influenced by the preparation method of transition metals-support material mixtures. It was found that the aligned MWCNTs are longer and more dispersible, compared with entangled MWCNTs. It was further found that the length of MWCNTs bundles could be controlled by varying the preparation conditions for both nanotubes and catalysts. The MWCNT-PMMA composites were prepared using both aligned and entangled MWCNTs through solution casting method. Aligned MWCNTs were found to give the composite higher conductivity, which might be attributed to long length and high dispersibility. In addition, the longer the MWCNT bundle is, the higher conductivity the MWCNT-composite shows.

## Poster Board | 268

### Computational studies on carbon nanotube-metal nanoparticle interactions

**Antti Tolvanen**, *University Of Helsinki, Materials Physics Division* | **Arkady Krasheninnikov**, *University Of Helsinki, Materials Physics Division; Aalto University, Laboratory of Physics*

Lack of exact control of the chirality in nanotube growth is currently the biggest obstacle on the way to carbon nanotube based commercially available nanoelectronic devices. In order to reach effective and controlled production of carbon nanotubes it is essential to fully understand current fabrication processes. Currently the most used method is chemical vapour disposition (CVD), where the diameter of the produced carbon nanotubes can be controlled by the size of metallic catalyst particles. In situ transmission electron experiments on single walled nanotube growth show both surface and bulk diffusion of carbon in catalytic metal nanoparticles.
We use classical molecular dynamics simulations with analytical bond-order potential and ab initio methods to study the energetics on carbon interstitials inside the nanoparticles and as ad-atoms on the surface. We show that geometry of the nanoparticle has an effect on the interstitial energetics and that nanotube growth can be explained in certain cases by bulk diffusion as observed in experiments. In addition to their appearance in nanotube growth, nanotube-nanoparticle interfaces can be created IN SITU using electron irradiation. These interfaces could be used as the link between carbon nanotubes device and macroscopic world. We present our recent computational results explaining how these interfaces are created and why is the defect production by electron irradiation an integral part of this process.

## Poster Board | 270

### Mass Production of Sub-Millimeter-Long CNTs by Semi-Continuous Fluidized-Bed CVD

**Dong Young Kim**, *Department of Chemical System Engineering, The University of Tokyo, Japan* | **Asuka Tashiro**, *Department of Chemical System Engineering, The University of Tokyo, Japan* | **Shunsuke Ueda**, *High-performance Materials Development Center, Hitachi Chemical Co., Ltd., Japan* | **Hisashi Sugime**, *Department of Chemical System Engineering, The University of Tokyo, Japan* | **Kei Hasegawa**, *Department of Chemical System Engineering, The University of Tokyo, Japan* | **Toshio Osawa**, *Department of Chemical System Engineering, The University of Tokyo, Japan* | **Suguru Noda**, *Department of Chemical System Engineering, The University of Tokyo, Japan*

Millimeter-long carbon nanotubes (CNTs) can now be grown as vertically aligned forests on catalyst supported substrates by chemical vapor deposition (CVD) [1]. However, such methods have unsolved problems of the limited productivity and catalyst deactivation. To solve the former problem, we coupled the forest growth with the fluidized bed [2]. Owing to the huge volume-to-surface ratio of 0.5-mm-sized ceramic beads, a productivity of 0.23 g-CNTs/ 50 mL-reactor/ 10 min was achieved at a carbon yield of 65 at.%. Especially, sputtered catalysts yielded 0.5-mm-long, 99at%-pure, single-walled CNTs. Here, we report our recent achievements on the improved productivity by solving the latter problem, i.e. catalyst deactivation. First, Al2O3 underlayer and Fe particles were deposited on the Al2O3 beads by CVD in 1-2 min. Next, CNTs were grown for 10 min by CVD. Then, CNTs were separated from the beads in 1-2 min by vigorously mixing the beads by a carrier gas. And finally, residual carbon on the beads was burned off in ~ 5 min. All these processes were carried out only by switching the gas flow at a fixed temperature of 820 degree C. The catalyst re-support method efficiently overcame the catalyst deactivation problem and estimated repeatable for ~ 10,000 times. By using a 50-mL reactor, we can now produce 5 g CNTs per 20 cycles in 10 h at a carbon yield over 70%. [1] S. Noda, et al., Jpn. J. Appl. Phys. 46, L399 (2007). [2] D. Y. Kim, et al., CT-05 in NT09, Beijing, China, June 22, 2009.

## Poster Board | 272

### Carbon nanotubes Nanocrystalline diamond composite material

**Clément Hébert**, *CNRS Neel Institute,CEA/INAC/SPrAM, Joseph Fourier University (Grenoble,France)* | **Sebastien Ruffinatto**, *CNRS Neel Institute,CEA/INAC/SPrAM,INP,France* | **David Eon**, *Joseph Fourier University (Grenoble, France), CNRS Neel Institute* | **Franck Omnès**, *CNRS Neel Institute,France* | **Pascal Mailley**, *Joseph Fourier University (Grenoble, France), CEA/INAC/SPrAM*

The development of implantable electrodes for brain electronic connection is an ongoing tremendous project that interests many labs. However the development of biocompatible and stable materials enabling neurons interfacing is still challenging. Carbon nanotubes (CNTs) were proved to be very promising materials to undergo these features [SUCAPANE09]. Nevertheless the polemic linked to its possible toxicity leads to find substrats on which carbon nanotubes can be strongly bonded in order to avoid spreading within the brain. To reach this goal we grew carbon nanotubes on nanocrystalline and microcrystalline diamond films. Hence our study mainly focuses on the growth process and the development of new characterizations to test the adhesion of CNTs on diamond. Carbon nanotubes were grown on diamond films using in a Hot Filament CVD reactor (HFCVD) under C H4 -H2 atmosphere from several nanodispersed catalysts (Co,Pd,Al,Ni) obtained through metal thin layer dewetting. We studied the influence of the nature and the thickness of these catalysts on CNTs density, type and adhesion. We also investigated the contribution of filament temperature and the ratio CH4/H2 to the growth. We characterized the samples with FEG-SEM to roughly evaluate the type and the density of carbon nanotubes that were grown. We also use Raman spectroscopy to control the quality and the nature of the CNTs. Finally we utilized AFM to perform force curve in order to determine the minimal adhesion force of CNTs on diamond films. In parallel we essayed microfluidic characterizations to get information on the adhesion of the whole CNTs carpet.

## Poster Board | 274

### Targeted growth of single-walled carbon nanotubes for nanosensor devices

**Miroslav Haluska**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Lukas Durrer**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Thomas Helbling**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Matthias Muoth**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Moritz Mattmann**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Kiran Chikkadi**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Tobias Suss**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Cosmin Roman**, *Micro and Nanosystems, ETH, Zurich, Switzerland* | **Christofer Hierold**, *Micro and Nanosystems, ETH, Zurich, Switzerland*

We are focusing on the application of SWNTs in pressure and gas sensors. The application requests a targeted fabrication of nanotubes with preferably well controlled characteristics. The Schottky barrier at the interface of the metal and the SWNT depends - among other factors - on the diameter of the nanotube [1]. To decrease the barrier, the CVD growth of SWNTs is targeted towards a diameter of ~2 nm, which is optimal for Pd contacts. Diameter selected catalyst particles are prepared by the loading of apoferritin protein with iron followed by gradient ultracentrifugation. Mass separated catalyst precursors are adsorbed on a patterned Si/SiO2/photoresist substrate. After removing the photoresist, samples are heated in air at 850°C to remove the ferritine protein shell. After the reduction of iron oxide in hydrogen atmosphere, SWNTs are grown at 850 °C in 300 mbar H2/CH4 [2]. Alternatively, acetylene is used as a carbon source gas for temperature sensitive substrates and SWNTs are then prepared at 700 °C. The metal-nanotube contact area is protected by an Al2O3 passivation film formed by atomic layer deposition. The devices are then characterized by AFM, electrical measurements, Raman spectroscopy and SEM. With the presented approach, ultra-small, highly sensitive SWNT sensors with low power consumption and long term stability are fabricated [3, 4]. [1] J. Svensson et al.: Nanotechnology 20 (2009) 175204. [2] L. Durrer et al.: Nanotechnology 20 (2009) 355601. [3] M.

Mattmann et al.: Appl. Phys. Lett. 94 (2009) 183502. [4] T. Helbling et al.: Nanotechnology 20 (2009) 434010.

## Poster Board | 276

### Synthesis and characterization of N-doped carbon nanotube with controlled tip shape

**Maria Luisa Garcia-Betancourt**, *Instituto Potosino De Investigación Científica Y Tecnológica (IPICYT)* | **Emilio Muñoz-Sandoval**, *Instituto Potosino De Investigación Científica Y Tecnológica (IPICYT)* | **Sofia Vega-Díaz**, *Instituto Potosino De Investigación Científica Y Tecnológica (IPICYT)* | **Juan Antonio Briones**, *Instituto Potosino De Investigación Científica Y Tecnológica (IPICYT)* | **Néstor Perea-López**, *Instituto Potosino De Investigación Científica Y Tecnológica (IPICYT)* | **Mauricio Terrones**, *Universidad Iberoamericana (UIA)*

In this work a systematic characterization of nitrogen doped carbon nanotubes (CNx) with controlled tip structure is presented. CNx were synthesized by chemical vapor deposition method using benzylamine as carbon and nitrogen source. The tip formation was controlled by pressure and flux conditions. These CNx nanotubes were characterized by scanning and transmission electron microscopy, thermal gravimetric analysis, Raman spectroscopy, X-ray diffraction analysis and vibrating sample magnetometry. Our results show CNx tubes with different diameters with a clear modification in the their "bamboo" like structure, showing tips of around 150 nm high, with an apex of around 20 nm that could contain open or filled compartments by Fe catalytic particle. Tip images were obtained by HRTEM, they show CNx with different tip shapes that could have catalytic particles at different sites. Additionally, these sharp tipped CNx were tested as electron field emitters and the tip formation mechanism was discussed.

## Poster Board | 278

### Effects of Water Addition on Single-Walled Carbon Nanotube Growth by Alcohol Gas Source Method in High Vacuum

**Takahiro Maruyama**, *Meijo University* | **Kuninori Sato** | **Shigeya Naritsuka**

Alcohol gas source method in an ultra-high vacuum (UHV) is effective to grow single-walled carbon nanotubes (SWNTs) at low temperature [1]. However, the yield has not been sufficient because of low growth pressure, especially in the growth at low temperature. In this study, for the purpose of increasing the yield, we investigated effects of water addition on SWNT growth at low temperature in the alcohol gas source method. SWNTs were grown on SiO2/Si substrates with Co catalysts at 400°C. The ethanol pressure was fixed at 1.0x10-4 Pa, while the water partial pressure was varied between 0 and 1.0x10-4 Pa. In addition, we varied the ethanol temperature to change the concentration of water vapor in the ethanol gas. The ambient gas was monitored by quadrupole mass analyzer and the grown SWNTs were characterized by SEM and Raman measurements. When the water pressure was 0.2x10-4 Pa, G band intensity became its maximum in the Raman spectra, while the SWNT yield decreased above 0.4x10-4 Pa. The SWNT yield enhancement was also observed by increasing the ethanol pressure from -10 to 70°C. Irrespective of the concentration of water vapor in the ethanol gas, the G/D ratios were more than 20 in the Raman spectra. These results indicated that proper water addition is effective to enhance SWNT yield in low temperature growth using the alcohol gas source method. We also compared the effect of water addition between ethanol source and hydrocarbon one and discussed the enhancement mechanism. [1] K.Tanioku et al., Diam. Relat. Mater. 17(2008)589.

## Poster Board | 280

### Role of the Molecular Structure of the Carbon Source in CNT Growth

**Mukul Kumar**, *Meijo University* | **Kaushik Ghosh**, *Meijo University* | **Yoshinori Ando**, *Meijo University*

Despite a huge experimental and theoretical research on carbon nanotubes (CNTs) worldwide, the CNT growth mechanism is not yet fully understood [1]. It is still debatable whether the molecular structure of the carbon source plays a significant role in the CNT growth or not. Majority of scientists think that, in the CVD temperature range of 600–800°C, any hydrocarbon will decompose into atomic carbon; so the molecular structure of the starting material is immaterial. In contrast, some researchers feel that, at the same temperature, different molecules will break in different manners; different radicals will have different dissociation energy, diffusivity and mobility on the catalyst particle; so they may affect the morphology of the resulting CNTs. Hence in the present study, N-doped CNTs were grown from two precursors: (i) from a cage-like carbon source: camphor using dimethylformamide as a nitrogen source; and (ii) from a linear-chain amino-hydrocarbon: octadecylamine as a dual source of carbon and nitrogen. And the study strongly suggests that the molecular structure of the precursor plays an important role in governing the structural properties of the resulting CNTs. The study is based on SEM, TEM, HRTEM, Raman, TGA and BET analyses. In all these characterizations, significant differences are noticed for the CNTs grown from the two carbon sources. These differences are explained in terms of the growth chemistry and nitrogen moieties. Reference [1] M. Kumar, Y. Ando, Chemical Vapor Deposition of Carbon Nanotubes: A Review on Growth Mechanism and Mass Production, J. Nanosci. Nanotechnol., 10(6), 3739 (2010).

## Poster Board | 282

### High-yield synthesis of carbon nanocoils using FeMgSnCo catalyst with Sn-O buffer layer

**Kaori Hirahara**, *Frontier Research Base for Global Young Researchers, Osaka University; Department of Mechanical Engineering, Osaka University* | **Yoshikazu Nakayama**, *Frontier Research Base for Global Young Researchers, Osaka University*

Composite particle of iron-, indium- and tin-oxides (Fe-In-Sn-O) is the effective catalyst for mass-production of carbon nanocoils (CNCs) by chemical vapor deposition (CVD)[1]. Recently, Fe-Mg-Sn-O catalyst is also found to be effective[2], and add of cobalt boosts the productivity. Fe-Mg-Sn-O and Fe-Mg-Sn-Co-O catalysts might be rather applicable to practical use in the viewpoint of cost-effectiveness, since no rare element is included. These catalysts, however, simultaneously produce by-product, which is a thick layer of graphitic materials including catalytic metals, between CNCs and substrate. This means large amount of carbon source gas and catalysts are still wasted. To solve this problem, we propose introducing SnO2 layer as a buffer between the catalytic particles and substrate. In this study, SnO2 layers were formed on Al2O3, SiO2, and Si3N4 substrates by spin-coating aqueous- or alcoholic-solution of SnCl4 and oxidation treatment. Fe-Mg-Sn-Co-O particles were then supported onto the substrates by the conventional wet process [1]. As the result of 15 minutes CVD with Fe-Mg-Sn-Co-O 600nm / SnO2 30nm thickness, the by-product layer drastically decreased. Alternatively CNC grew up to 65μm, >200% longer than the conventional method. It is supposed that additional supply of Sn from SnO2 layer prevented the catalytic particles from decreasing Sn with low melting point, which helped keeping appropriate elemental ratio for growing CNCs. Acknowledgement: This work was supported by Osaka Prefecture Collaboration of Regional Entities for the Advancement of Technological Excellence, JST. [1] N. Okazaki et al., J.Phys.Chem.B (2005) 109, 17366 [2] S. Kugimiya et al., US patent. WO/2010/005118, PCT/JP2009/062932, 2010-1-14.

## Poster Board | 284

### Structural changes and gas-sensing properties of phosphorus- and silicon-doped multi-walled carbon nanotubes

**Antal A. Koós**, *University of Oxford, Department of Materials, UK* | **Alison Crossley**, *University of Oxford, Department of Materials, UK* | **Frank Dillon**, *University of Oxford, Department of Materials, UK* | **Krisztián Kertész**, *Research Institute for Technical Physics and Materials Science, Hungary* | **László P. Biró**, *Research Institute for Technical Physics and Materials Science, Hungary* | **Nicole Grobert**, *University of Oxford, Department of Materials, UK*

Due to their exceptional properties carbon nanotubes (CNTs) are expected to have many applications, but for most products

CNTs with well defined properties at commercially viable price are needed. It is possible to tailor the electrical, mechanical and chemical properties of CNTs by replacing some atoms from graphitic carbon network with dopants. The doping with P and Si allows us to tailor the density of states and produce CNTs with new chemical properties. Both P- and Si-doped nanotubes are expected to work as very fast and sensitive chemical sensors, and they can be the building blocks of advanced electronic devices and composite materials. Unfortunately, both the controlled doping and large scale production of doped nanotubes are challenging. To the best of our knowledge there are only a few reports about production of P-doped nanotubes (sufficient quantities for further investigations are not readily available), while the large scale production of Si-doped CNTs was not reported yet. Herein we investigate the effect of reaction parameters on the structure of multi-walled CNTs produced via aerosol chemical vapour deposition technique from phosphorus and silicon containing precursors. Up to our knowledge we produced Si-doped nanotubes in high quantities for the first time. We were able to control the structure, diameter distribution, defect density and oxidation resistance of the nanotubes. Gas sensing properties of the doped nanotubes were also investigated. Our results can be used to produce nanotubes with well defined properties for electronic components, composite materials or high performance chemical sensors.

## Poster Board | 286

### Nanoscale Zirconia and Other Oxides as Non-Metallic Catalysts for Graphitization of Carbon and Growth of Single- and Multi-Wall Carbon Nanotubes

**Stephen Steiner III**, *Massachusetts Institute of Technology* | **Bernhard Bayer**, *University of Cambridge* | **Stephan Hofmann**, *University of Cambridge* | **Brian Wardle**, *Massachusetts Institute of Technology*

We present that nanoparticulate zirconia (ZrO2) catalyzes both growth of SWNTs and MWNTs by thermal chemical vapor deposition (CVD) and graphitization of solid amorphous carbon. We observe that silica-, silicon nitride-, and alumina-supported zirconia on silicon nucleates single- and multiwall CNTs upon exposure to hydrocarbons at moderate temperatures (750°C). Using in situ, high-pressure, time-resolved X-ray photoelectron spectroscopy (XPS) of these substrates during CNT nucleation and growth, we show that the zirconia catalyst neither reduces to a metal nor forms a carbide. Point-localized energy-dispersive X-ray spectroscopy using scanning transmission electron microscopy confirms catalyst nanoparticles attached to CNTs are zirconia. We also observe that carbon aerogels prepared through pyrolysis of a Zr(IV)-containing resorcinol-formaldehyde polymer aerogel precursor at 800°C contain fullerenic cage structures absent in undoped carbon aerogels. Zirconia nanoparticles embedded in these carbon aerogels are further observed to act as nucleation sites for multiwall CNT growth upon exposure to hydrocarbons at CVD growth temperatures. Our study unambiguously demonstrates that a non-metallic catalyst can catalyze CNT growth by thermal CVD while remaining in an oxidized state. Recent observations of growth from engineered zirconia nanoparticles and other oxides not reducible under CVD growth conditions will be presented. Considerations regarding yield, the role of defects, and the presence of hydrogen will be discussed. We believe characterization of the mechanism underlying CNT growth from oxides will aid in the engineering of optimized non-metallic catalysts for CNT growth on historically-challenging substrates such as carbon fiber and may offer a promising route towards shape- and chirality-control of CNTs.

## Poster Board | 288

### Study of the dewetting of a Fe film for single-walled carbon nanotubes growth by CVD

**Pierre Evellin**, *Onera, France; Cea (Grenoble, France)* | **Annick Loiseau**, *Onera, France* | **Raul Arenal**, *Onera, France* | **Jean Dijon**, *Cea (Grenoble, France)*

CVD synthesis route is the most promising technique for producing C-SWNTs at an industrial level. However, understanding and controlling the SWCNTs parameters such as diameter, chirality or metallic character is a tremendous prerequisite for any application in electronics. Several studies succeeded in changing the ratio metallic/semi-conducting SWCNTs [1,2] but without clear explanation of the observed selectivity. Among the different steps to be considered,the one related to the control of the size and chemical state of catalytic particles is of major importance as it is tightly linked to the SWNT diameter and chirality. Here we report on the formation mechanism of Fe catalytic particles issued from the thermal heating of a film deposited on a substrate. By using thin oxide membranes as substrates [3], we have inspected by direct TEM observations, the dewetting mechanism of the film as a function of various parameters: nature of the substrate, heating procedure and annealing temperature, environmental atmosphere. We show that first, the oxidation state of the film crucially impacts the dewetting process and the size distribution of the particles, and second, only reduced particles can be active for the nanotube nucleation. Finally,dewetting is found to occur more slowly on alumina than on silica, therefore favoring the formation of particles with a reduced size and a more uniform distribution. [1] Wei-Hung Chiang and R. M. Sankaran, Nature materials (Sept.2009) [2] A. R. Harutyunyan, et al., Science 326, 116 (2009) [3] M.-F. Fiawoo, Surface Science 603, 1115-1120 (2009)

## Poster Board | 290

### VANTA Nucleation, Growth, and Density Variations Measured by Pulsed CVD and in situ Reflectivity

**Jeremy Jackson**, *Center for Nanophase Materials Sciences, Oak Ridge National |Laboratory* | **Alex Puretzky**, *Center for Nanophase Materials Sciences, Oak Ridge National Laboratory* | **Gyula Eres**, *Materials Science and Technology Division, ORNL* | **Chris Rouleau**, *Center for Nanophase Materials Sciences, Oak Ridge National Laboratory* | **Karren More**, *SHaRE Facility, ORNL* | **David Geohegan**, *Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*

The density of vertically-aligned carbon nanotube arrays have been measured in real-time during continuous growth by chemical vapor deposition and found to decline up to 50% during the first 10 microns of height. Derivation of the evolution of nanotube array density during growth is described from in situ optical measurements of the array height and extinction coefficient. Ex situ Z-contrast scanning transmission electron microscope density analysis of sections of the arrays confirm this natural decline in array density with length and time. Using this real-time optical diagnostic technique, the response of array density to rapidly varying feedstock flux was explored using pulsed-CVD in fast flows at low pressures. Acetylene pulses of ~0.5 s duration were found to induce the growth of distinct ~1-2 micron-long layers within which densities varied up to ~ 200%. This highly responsive flux-dependence to the density of the arrays, along with the described optical density measurement technique, is shown to provide a pathway not only to monitor the density of VANTAs as they grow but to synthesize interesting new multilayered array architectures with regions of controllable length and density variations. Synthesis science sponsored by the U.S. Dept. of Energy Office of Science, Basic Energy Sciences, Division of Materials Science and Engineering. Characterization facilities at CNMS and ShaRE sponsored by DOE-BES, Division of Scientific User Facilities.

## Poster Board | 294

### QM/MD Simulations of Single-Walled Carbon Nanotube Nucleation on Transition Metal Catalysts

**Alister Page**, *Fukui Institute for Fundamental Chemistry, Kyoto University, Japan* | **Honami Yamane**, *Fukui Institute for Fundamental Chemistry, Kyoto University, Japan* | **Stephan Irle**, *Institute for Advanced Research and Department of Chemistry, Nagoya | University, Japan* | **Keiji Morokuma**, *Fukui Institute for Fundamental Chemistry, Kyoto University, Japan; Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, USA*

Transition-metal-catalyzed synthesis of SWCNTs is now a routine process on industrial scales. Nevertheless, the precise mechanisms underpinning many facets of SWCNT nucleation are either in question, or yet to be understood entirely. We report here a systematic investigation of SWCNT nucleation on Fe-/Ni-catalyst nanoparticles using QM/MD methods. Our simulations suggest that SWCNT nucleation occurs according to the following sequence: 1. polyyne chains are formed on the catalyst following the diffusion of atomic carbon; 2. these polyyne chains coalesce, preferentially forming a 5-membered ring as the SWCNT “nucleus”; 3. polyyne chains bonded to this nucleus interact, resulting in further ring condensation and ultimately nucleation [1]. Our simulations indicate that this mechanism is independent of a number of pertinent factors, such as catalyst composition, diameter and reaction temperature. However, the kinetics of nucleation are enhanced using Ni, a fact that is consistent with reported SWCNT growth rates [2, 3]. The origin of the carbon source (whether carbon is deposited on the catalyst, or precipitates from a metal-carbide phase) also has no effect on nucleation. With respect to SWCNT nucleation from a metal-carbide precursor, it is observed that carbon precipitation from the bulk to the catalyst surface occurs within several hundreds of picoseconds. Our simulations therefore suggest that supersaturation in small metal particles occurs at lower carbon/metal ratio than usually assumed. [1] Y. Ohta et al., ACS Nano 2009, 3, 3413. [2] A. J. Page et al., Carbon, Submitted. [3] Z. P. Huang et al., Appl. Phys. A, 2002, 74, 387.

## Poster Board | 296

### Individually-dispersed SWNTs solutions and enrichment of (8, 4) SWNTs solutions with polysaccharides

**Bee Eng Mary Chan**, *Nanyang Technological University* | **Liangyu Yan**, *Nanyang Technological University*

Various neutral pH water-soluble chitosan derivatives and heparin sodium salt were investigated for dispersing single-walled carbon nanotubes (SWNTs). Chitosan (CS) can disperse SWNTs well, but only in acidic pH condition. Our two novel derivatives, O-carboxymethylchitosan (OC) and OC modified by poly(ethylene glycol) at the -COOH position (OPEG), were able to produce highly effective debundling and dispersion of SWNTs in neutral pH aqueous solution. Individual nanotubes present in the dispersions were confirmed with transmission electron microscopy (TEM), atomic force microscopy (AFM), photoluminescence (PLE) and UV-vis-NIR spetroscopy. The solubilities of individually dispersed SWNTs in neutral water are 0.021 and 0.032 g/L for OC and OPEG, respectively, which are comparable to 0.038 g/L for SWNTs using CS in acetic acid. When heparin sodium salt was used as dispersant for CoMoCAT nanotubes, (8, 4) tubes were extracted and enriched in supernatant by heparin. In pristine CoMoCAT nanotubes, (6, 5) nanotubes was predominant which have smaller diameter than (8, 4) nanotubes. After threefold extractions, the composition percentage of (8, 4) tubes increased from 7% to 60%, which was calculated from PLE intensity. We also apply computer modeling to verify that heparin has lower binding energy with (8, 4) nanotubes compared to the four other kinds semiconducting nanotubes in CoMoCAT nanotubes. (8, 4) nanotubes enrichment solutions were successfully used for fabrication of network field-effect transistors, confirming the easy removability of heparin.

## Poster Board | 298

### Effect of the laser heating of nanotube nuclei on the nanotube type population

**Pavel Nikolaev**, *Sungkyunkwan University* | **William Holmes**, *The University of Texas at Dallas* | **Edward Sosa**, *ERC Inc. / NASA Johnson Space Center* | **Peter Boul**, *ERC Inc. / NASA Johnson Space Center* | **Sivaram Arepalli**, *Sungkyunkwan University*

Many potential applications of carbon nanotubes are expected to benefit from the availability of single wall carbon nanotube materials enriched in metallic species, and specifically arm-chair nanotubes. The present work focuses on the modification of the pulsed laser vaporization technique to selectively produce certain carbon nanotube structures. Nanotube nuclei were “warmed-up” with an additional laser pulse, timed to coincide approximately with the nucleation event. The effect of the second laser on the carbon vapor temperature was studied by emission spectroscopy. Nanotube type populations with and without warm-up were compared by means of photoluminescence and Raman spectroscopy. It was found that the warm-up of nanotube nuclei with a laser pulse has a noticeable effect on the nanotube population. The intensity of spectral features of both metallic and semiconducting nanotubes with large chiral angles increased, while small chiral angle nanotubes decreased or remained unchanged. The time delay between ablation and warm-up laser pulses leading to the largest population shifts is 0.25 ms in case of Rh/Pd catalyst and 500 _?_ in case of Co/Ni catalyst. This is consistent with earlier nanotube nucleation expected for less volatile Rh/Pd catalyst. This experiment demonstrates that nanotube population during PLV synthesis can be manipulated in a controlled fashion.

## 15:30-17:00 Poster take-down (for Poster Sessions 1-3)

# Thursday, July 1

## 7:00-8:30 Poster set-up (for Poster Sessions 4-6)

## 10:01-11:30 Poster Session 4

### Poster Board | 1

### Negative Differential Resistance in Carbon Nanotube Field-Effect Transistors

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First demonstration of negative differential resistance (NDR) in an electronic device was made during the seventies in a GaAs double barrier structure[1]. There is a great interest for NDR in decreasingly smaller devices, motivated by the desire to reach high device integration densities. Another driving force is the fact that the capacitance of the NDR element is proportional to its size and if being too large it restricts the accessible device characteristics. Recently, there have been emerging carbon nanotube (CNT) devices that exhibit NDR in their electrical characteristics. In these devices, so far, the appearance of NDR has been uncontrolled and not suitable for mass production. Here we describe a lithographic method for controlled and reproducible introduction of NDR in CNT field - effect transistors (FETs). Our approach opens a possibility for a new class of nanoscale electronic devices using NDR: fast switching elements[2,3], nanoscale amplifiers[4], and high frequency oscillators[5] which operate well into the THz domain. [1] Chang, L. L.; Esaki, L.; Tsu, R. Appl. Phys. Lett. 1974, 24, 593-595. [2] Haddad, G. I.; Mazmunder, P. Solid-State Electron. 1997, 41, 1515-1524. [3] Mazumder, P.; Kulkarni, S.; Bhattacharya, M.; Jian Ping Sun; Haddad, G. Proceedings of the IEEE 1998, 86, 664-686. [4] Laskar, J.; Ketterson, A. A.; Baillargeon, J. N.; Brock, T.; Adesida, I.; Cheng, K. Y.; Kolodzey, J. IEEE Electron Device Lett. 1989, 10, 528-530. [5] Dragoman, D.; Dragoman, M. Physica E 2004, 24, 282-289.

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### Electrokinetic's methods in the group microelectronics process of carbon nanotubes sensors production

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The main technological problems connected with integrating nanotubes into the functional devices and structures. Electrokinetics methods like electrophoresis potentially allow us to resolve it. In this work we present the results of employing electrophoresis in the tasks of investigating carbon nanotubes in electronic applications; we also describe the main trends of electrophoresis usage in the purification and separation processes of carbon nanotubes. In this work the deposition of carbon nanotubes between electrodes was performed using both a direct and an alternating current. Carbon nanotubes obtained by the method of arc discharge were preliminarily diluted in 10 mL of 2-propanol for several hours in an ultrasonic bath. Then, 1 mkL of the resulting solution was applied to the device and it was hooked up to the direct or alternating voltage sources limiting electrodes. After the process stopped, the alcohol was removed. The structures of thin conductive strips with period of 2 mkm and thickness of 50 nm was produced by the methods of traditional lithography on oxidized silicon wafer 3 inch in diameter. Varying the geometry of electrodes and the electrophoresis parameters we able to control the nanotubes deposit structure from single nanotubes to networks and films with predefined densities of nanotubes. In this work the main results on application of electrophoresis in the tasks of nanoelectronics based on carbon nanotubes were shown, also the promising trends of its usage were considered.

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### Silver nanowires as flexible, transparent conductors: Controlling network conductivity through nanowire geometry

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Thin transparent conducting films are critical for building many optoelectronic devices and components. Such films are usually made from doped metal oxides such as Indium Tin Oxide (ITO), which shows major drawbacks such as cost, brittleness and high temperature processing used in its production. We have prepared thin, flexible, transparent, conducting films from aqueous dispersions of silver nanowires (1). We obtained a sheet resistance of < 1 Ohm / sq for a film with optical transmittance (550nm) of 92 %. Those results make silver nanowires a possible replacement for ITO. In order to fully exploit such applicable properties the factors controlling the film conductivity must be understood. These films exhibit a transition from network to bulk-like DC conductivities at thicknesses of ~160nm(1). By measuring the DC conductivity above this saturation point for a selection of nanowires with lengths, L, and diameters, D, varying from 51nm to 105nm and 7.1µm to 44µm respectively we expect to see the DC conductivity vary with as L(D^n) where -2>n>-4. 1.De et al. Silver nanowire networks as flexible, transparent, conducting films: extremely high DC to optical conductivity ratios. ACSNano 2009, vol.3, no.7, 1767-1774

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### Sorted Semiconducting Single Wall Carbon Nanotube Films for Gas Sensors : A Comparative Study

**Olivier Ducloux**, *ONERA DMPH-CMT* | **Yann Battie**, *LEM CNRS-ONERA* | **Philippe Thobois**, *ONERA DMPH-CMT* | **Olivier Le Traon**, *ONERA DMPH-CMT* | **Annick Loiseau**, *LEM CNRS-ONERA*

We present in this paper a gas sensor dedicated to the detection of traces of gaseous pollutants in high temperature environment. The presented sensor consists of a patterned SWCNT film deposited on TLM (Transmission Line Method) electrodes. TLM is a common and reliable technique to simultaneously extract the contact resistance and the sheet resistance from electrical measurements. The structure is made of a silicon substrate covered with a 500nm thick SiO2 layer to provide electrical isolation, comprising 80nm thick Pt electrodes. The carbon nanotube films are obtained by filtration of a suspension of SWCNT through a nitrocellulose membrane, then transferred on the electrodes and released by dilution of the membrane. Prior to deposition, the semi-conducting nanotubes are sorted out from the initial suspension by ultra-centrifugation in a density gradient. Several iterations of the sorting procedure provide a good separation of the semi-conducting nanotubes from the metallic ones. Two types of films are then studied: unsorted films, including semi-conducting and metallic ones, and sorted semi-conducting nanotube films. The characterization setup is composed of a chamber, enabling pressure and temperature control during the conductivity measurements, in addition to the fine control of the gaseous environment of the studied sensor. First of all, the effect of the stabilization annealing on the sensors (prior to gas exposure) is presented. The response to different gas concentrations, at ambient and high temperatures, is then presented. Sensing results issued using the TLM method, obtained on sorted semi-conducting and unsorted SWCNT films are finally compared.

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### Large-scale, CMOS-compatible, bottom-up integration of chirality-sorted carbon nanotubes

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To realize the full potential of SWNTs, it is essential to integrate them into existing microelectronic products and techniques. SWNTs of a particular type/chirality need to be assembled at specific locations and orientations in lithographic circuits at 100% efficiency. SWNTs are sorted to single-chirality by polymer wrapping. They are enriched to high-purity in semiconducting species using density-gradient ultracentrifugation. SWNTs and graphene can be assembled at ultra-large-scale integration densities using dielectrophoresis (DEP), which is self-limiting to one SWNT per device. By adapting DEP for sorted solutions, we assemble SWNTs of specific chirality or electronic type at 100% yield. DEP is the only CMOS compatible route to simultaneously assemble SWNT devices in multiple orientations. Pre- and post-processing steps to extract high performance from such devices are also described. In addition to applications, understanding fundamental SWNT properties also depends on the ability to study them specifically. We perform multiple measurements on identical SWNTs and correlate interesting features. For instance, we demonstrate a strong correlation between D-peak in Raman spectroscopy, dark-exciton peaks in photoluminescence spectroscopy and low conductance and mobility in electron transport measurements. Vijayaraghavan, A.; et al., Toward single-chirality carbon nanotube device arrays. ACS Nano, In press Ganzhorn, M.; Vijayaraghavan, A.; et al., Large-scale, CMOS-compatible integration of high-performance semiconducting single-wall carbon nanotube devices. Submitted Vijayaraghavan, A.; et al., Dielectrophoretic Assembly of High-density Arrays of Graphene Devices for Rapid Screening. ACS Nano 2009, 3, 1729 Vijayaraghavan, A.; et al., Ultra-Large Scale Directed Assembly of Single-Walled Carbon Nanotube Devices. Nano Letters 2007, 7, 1556

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### Molecular vibration sensor via transport measurements in carbon nanotube

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Transport properties of armchair and zigzag carbon nanotubes (CNTs) coupled locally to a single optical phonon mode were studied under the presence of an applied bias. The purpose is to propose an ideal molecular nano-sensor device described by a simple theoretical scenario using a _?_-band tight-binding approach. The transport results show that the characteristic molecular vibration energy _?_ can be measured from the transmission coefficient and the differential conductance spectra. Also, by analyzing the slopes of the characteristic curves of current versus bias voltage one may study the effects of the electron-phonon coupling energy on the electric transport. Despite of the subtly of the molecular vibrations induced effects on the transport responses, the state of the art in experimental measurements indicates that they may be measurable.

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### Tailor-Made Carbon Nanotube Emitters: Combinatorial Searching for Emitters and their Implant for End-Uses

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On universal application of carbon nanotube (CNT) emitters and usage of soft-electron beam, the following issues: (1) scale-up probability of CVD reactors, (2) glass tolerability in CVD processes, (3) throughput (direct and rapid implementation without posttreatments), (4) practical field emission (FE) properties and (5) controllability of emitter morphologies, have to be concerned. 1-second synthesis of micrometer-tall CNTs through the pulse-current C2H2-CVD under atmospheric pressure [1] and fabrication/ evaluation of the line-patterned emitter arrays showing a practical operation voltage [2] provide prospects answering (1) – (4). Combinatorial masked deposition of catalysts [3] and FE evaluation for the obtained CNT-libraries [4] accelerates searching for CNT-types, -morphologies and number densities of emitters desired in end-uses. This approach augments (5) controllability of emitter morphologies (height, inter-space, sharpness). Here we report our current status in tailor making of self-organized CNT-emitters based on the physico-chemical and practical perspectives built up through the study on growth mechanism and device fabrication [1-4]. [1] S. Noda et al., NT09 (Beijing), p. 100 (2009). [2] Y. Shiratori et al., Nanotechnology 20, 475707-1-7 (2009). [3] S. Noda et al., Carbon 44, 1414 (2006). [4] Y. Shiratori et al., J. Phys. Chem. C 112, 17974-17982 (2008).

## Poster Board | 22

### Fabrication and evaluation of network single walled carbon nanotubes biosensors

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Single-walled carbon nanotubes (SWNTs) have been studied due to their potential applications in various fields, such as field-effect transistors, flexible electrodes, chemical sensors and probe tips. Especially, the electrical biosensor has shown higher sensitivity and great promise in label-free detection systems and nano-scale devices. In this work, we fabricated the highly sensitive protein sensor of novel structure which consists of a thin gold island (20 nm) on SWNT domains between electrodes because of having a critical thickness of metal for Schottky contact. The proteins immobilized by gold-thiol interaction on the gold island instead of on the SWNT side wall. The advantages of the well-defined immobilization method of protein and increased Schottky barrier area result in detecting at 1 pM concentrations

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### Hydrogen sensing with chirality sorted single walled carbon nanotubes

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The work function of Palladium is known to be sensitive to hydrogen by the formation of a surface dipole layer. An approach to detect such a layer is based on the formation of a Schottky barrier between the Palladium metal and a semiconductor. Here, we study the hydrogen sensitivity of Schottky-barrier field effect transistors (SB-FET) from (n,m)-sorted semiconducting single-walled carbon nanotubes (SWNT) in contact with Pd electrodes. Single chirality SWNTs in solution were obtained by polymer-mediated sorting and assembled to SB-FETs by low-frequency dielectrophoresis. . We observe for devices from (9,7) nanotubes a superior 100 fold change in the current at 100 ppm H2, but no sensitivity for devices from (6,5) nanotubes. The effect can be rationalized by a spillover of atomic hydrogen onto small diameter nanotubes and curvature dependent chemisorption. We also observe that long-term sensitivity is only achieved if the gate voltage is inverted periodically. Under constant gate bias, the sensitivity reduces with time, which we relate to gate screening by accumulated charges in the substrate.

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### Improvement of SWCNT-TCF characteristics by surface treatment of substrate

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This experiment was progressed to improve the SWCNT-TCF characteristics by applying various pre-treatments on PET substrate. The characteristics of SWCNT-TCF; resistance, transparency, adhesion; were improved by pre-treatment of substrate with chemical and physical method. In O2 plasma pre-treatment, the surface energy of PET increased from 40mJ/m2 to 75mJ/m2, which resulted that sheet resistance was decreased without changing light transparency and the amount of coating solution used to reach the same range of sheet resistance was reduced by 30%. In case of polyelectrolyte pre-treatment, the sheet resistance was more reduced than without pre-treatment. It showed that the characteristics of SWCNT-TCF were more improved when the surface has more negative surface potential. Also in adhesion test, it showed best adhesion property on PET substrate that treated by polyelectrolyte.

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### Hybrid CMOS logic inverter with individual single-walled CNTFET and ZnO FET

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The growth of single walled carbon nanotubes (SWCNT) and ZnO nanowires, has opened up avenues of further research based on the integration of these two different technologies. The p-type and n-type behaviour observed from SWCNT field effect transistors (FETs) and ZnO FETs have been exploited to fabricate a novel hybrid CMOS inverter on a 200nm-thermal-grown SiO2. SWCNTs and ZnO nanowires were in-situ grown on the same substrate with Fe/Mo and Au catalysts respectively. Pd and Nb contacts were sputtered for the p-type and the n-type FET respectively. These metals provide Ohmic contact whilst reducing the power dissipation. With a channel length of 500nm the output current of the SWCNT FET was 0.2μA. The on/off current ratio was 5 orders of magnitude with field effect mobility of 40cm2V-1s-1. The ZnO FET had a channel length of 600nm and the diameter of the nanowire was 60nm. The observed output current was 0.1μA with on/off ratio close to 3 orders of magnitude and the field effect mobility was found to be 120cm2V-1s-1. The logic gate device has a gain near to unity and it operates in the range of 0 to 2V. All measurements were conducted at room temperature. In spite of the relatively low mobility in the in-situ grown long channel SWCNT, these results verify that SWCNTs and ZnO nanowires can be incorporated on the same substrate to fabricate relatively low cost large scale integrated circuits. Results show that the extracted mobility is limited by contact resistance to the SWCNT.

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### Characterization of surfactant-assisted single walled carbon nanotube suspensions and fabrication of transparent conductive films

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Single walled carbon nanotubes (SWCNTs) have been commonly dispersed in water with an aid of surfactants prior to forming transparent conductive films. This study has quantitatively evaluated the effects of several anionic and cationic surfactants on the dispersion of purified SWCNTs in terms of dispersibility in water and electrical conductivity of SWCNT network films. The dispersibility of surfactants in an aqueous SWCNT solution was assessed with the amount of SWCNTs dispersed, the content of a surfactant required to suspend SWCNTs, and the long-term stability of dispersions. The absorption coefficient was calculated by using UV-Vis NIR spectroscopy to measure the concentration of SWCNTs in an aqueous solution. It was found that sodium dodecylbenzene sulfonate (SDBS) among many surfactants used was best in dispersing SWCNTs in water. Transparent conductive networks of SWCNTs were fabricated by air-spraying onto a PET substrate. The highest ratio of dc to optical conductivity for each film was observed to be DC/Op = 23.1 upon nitric acid treatment of the SWCNT film fabricated with the SDBS-stabilized dispersion. The doping of nitric acid was identified by UV-VIS NIR and Raman spectroscopy, likely improving the electrical conductivity of the SWCNT films.

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### Field Emission Properties of Nanotubes for Application in High Efficiency Lighting

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Energy efficiency has been at the top of the global agenda recently, as global warming becomes apparent, and energy supplies more unstable. Lighting contributes significantly to global consumption of energy (ca. 20%), and hence any improvement in the efficiency of lights would help reduce CO2 emissions. Energy saving bulbs already exist in the form of compact fluorescent lighting. However, as this method uses thermionic emission, some energy is lost as heat. A florescent light that uses only field emission (FE) would therefore improve bulb efficiency. CNTs have excellent FE properties, due to their high aspect ratio and depressed work function. The work function can be further tailored through doping. We investigated the FE emission properties of individual, and films of pure, N, and B-doped CNTs produced via aerosol CVD as this method is relatively cheap and scalable. SEM, TEM and Raman spectroscopy were employed to study the morphology, defect density and arrangement of CNTs produced. The relationship between FE properties and the various types of samples produced (such as doped CNTs, CNTs with different defect densities etc.), is reported. Further work shall concentrate on the application of CNT emitters into high efficiency lighting.

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### Carbon nanotubes arrays as contacts for p- and n-type organic field-effect transistors

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**Carla M Aguirre**, *Département de Chimie, Université de Montréal, Canada* | **Richard Martel**, *Département de Chimie, Université de Montréal, Canada*

The outstanding electrical and mechanical properties of carbon nanotubes combined to chemical inertness, thermal stability and high aspect ratio make them ideal materials for electronics. Here we explore the performance of carbon nanotube array electrodes to organic thin-film transistors (OTFT). We demonstrated that these arrays electrodes provide effective hole and electron injection with pentacene and PCBM organic semiconductors, respectively. In comparison to metal contacts, OTFT with nanotube electrodes display a close to ideal injection behavior, high FET mobility and fast switching characteristics. The exceptional injection efficiency of nanotube electrodes represents a breakthrough in organic electronics and opens exciting scenarios for OTFT. CNT array electrodes applied to ambipolar OTFT (with both electron and hole injection) will be presented.

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### Point-functionalized carbon nanotubes for electrical detection of single enzyme activity

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Carbon nanotubes (CNTs) with engineered point defects are an extremely promising system for studying chemical reactions and biological activity at the single-molecule level. Here we report theoretical and experimental progress towards the goal of detecting enzymatic turnover events at unprecedented temporal resolution using CNT point defect devices. Our approach follows the pioneering work of Goldsmith et al. and utilizes a single charge-sensitive point defect in an otherwise metallic CNT. The electrostatic environment of the point defect modulates the resistance of the entire device. We have used computational methods to determine the electrostatic signature of single enzyme activity and show that these electric fields exceed background noise levels in existing point defect devices. Our point-defect CNT devices have been fabricated using an AFM-based electrical technique to induce local damage in individual, electrically contacted CNTs. Electric field sensitivity and intrinsic noise levels have been characterized in biological buffer solutions and sensitivity to single ion binding events has been demonstrated. We will discuss prospects for extending this work to study single enzymes.

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### Orbital motions of electrons and induced magnetic fields in defected carbon nanotubes

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When defects exist in a metallic carbon nanotube, the current-flow under finite bias voltage is expected to have characteristic patterns depending on the nature of the defects. Using first-principles calculations, we investigate the current-density distribution and the induced magnetic fields in defected carbon nanotubes. The current-density loops are generated around the defects by the interference between conducting states and quasibound states at energies close to conductance dips originated from resonant backscattsering. Directions of the loop current at above and below the resonant energy are opposite with its magnitude being exactly zero at the resonance. The current-density loops produce magnetic fields penetrating the tubular surface in the near-field region and decaying like a magnetic dipole in the far-field region. Oscillating magnetic fields can be generated by alternating the loop directions with a time-modulated gate-voltage, thereby making experimental detections feasible. We propose that the defected nanotube may be used as a probing tip of atomic force microscopy to measure minute magnetic fields with a nanometer-scale resolution.

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### Electronic transport in individual carbon nanotubes under extreme conditions

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Carbon nanotubes can be used to design numerous types of nano-electromechanical systems (NEMS), such as mass detectors, oscillators, strain gauges... However, the field of high-pressure remains mainly unexplored from an experimental point of view, though it features some interesting and specific effetcs, such as structural transitions implying the nanotube cross section. This lack of experiment is mainly due to the difficulty of carrying out transport measurements under high-pressure on one individual nanotube. Here we show how we have been able to carry out such experiments. Results are presented for semiconducting and metallic nanotubes. We show that these measurements allow a good understanding of pressure effects, should they come from the nanotube themselves or their environment. In particular, we evidence a signature for the structural transition in the multiwalled nanotube, as well as the tuning of its transistor type. We also explain how a gold-nanotube junction can serve as a nanometric and sensitive high-pressure gauge.

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### Influence of defects on the Raman spectra of individual semiconducting single walled carbon nanotubes

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The introduction of defects into single walled carbon nanotubes (SWCNTs) can lead to new interesting properties. Therefore understanding how the defects can change the electronic properties of nanotubes may open a route towards engineering new electronic devices by controlling or creating defects. Here we use Raman spectroscopy to study the effect of defects on Raman spectra of individual semiconducting SWCNTs. These defects were intentionally created by Ar plasma on a part of originally defect-free individual nanotubes. This allowed us to investigate the changes in the electronic structure of a particular SWCNT by creation of the defects. We show that not only the increased D band is a signature of defects in Raman spectra of carbon nanotubes. The creation of defects also caused a significant decrease of the intensity of other Raman features. In addition we investigate the changes of the resonance window of a nanotube in the presence of defects. It is shown that defects lead to a broadening of the Raman resonance profile and also to a decrease of the resonance profile intensity maxima.

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### Upper bound for the conductivity of nanotube networks

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Films composed of nanotube networks have their conductivities regulated by the junction resistances formed between tubes. Conductivity values are enhanced by lower junction resistances but should reach a maximum determined by the network morphology. By considering ideal contacts between nanotubes we calculate the upper bound for the conductivity of such films, a useful tool to avoid overoptimistic expectations for their transport properties. Compared to real measurements, our results indicate how much room there is to improve the junction resistance. Highest measured conductivities reported so far are approaching this limiting value, suggesting that further progress lies with nanowires other than nanotubes [1]. [1] L. F. C. Pereira, C. G. Rocha, A. Latge, J. N. Coleman and M. S. Ferreira, Appl. Phys. Lett. 95, 123106 (2009)

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### Physical studies on individual carbon nanotubes

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From well dispersed suspensions of carbon nanotubes we fabricate devices based on individual nano-objects (individual single walled carbon nanotubes, individual double walled carbon nanotubes or small bundles) contacted in transistor geometry. Each device has been studied by combined electronic transport, resonance Raman spectroscopy and AFM measurements. From electrical studies on Raman identified nanotubes, we are discussing the relation between structure, Raman signatures and electrical characteristics and give preliminary interpretations of some unusual transfer characteristics measured. The role played by the gaseous and electrostatic environment on the device electrical behavior, the nanotube Raman signatures and the electron-phonon coupling will also be presented and discussed.

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### Experimentally Determined Precise Electronic States of Individual (n,m) Single Walled Carbon Nanotubes

**Naotoshi Nakashima**, *Kyushu University; JST-CREST* | **Yasuhiko Hirana**, *Kyushu University* | **Yasuhiko Tanaka**, *Kyushu University* | **Yasuro Niidome**, *Kyushu University*

Ever since the discovery of carbon nanotubes (CNTs), many groups have endeavored to understand the fundamental properties of the CNTs. The redox properties (i.e. electronic densities, the Fermi levels, redox potentials) of single-walled carbon nanotubes (SWNTs) are related to the structures of SWNTs that have a specified diameter and chirality angle uniquely related to a pair of integers (n,m); the so-called chiral indices. Many attempts have been made to determine the electronic properties of SWNTs using scanning tunneling spectroscopy, redox titrimetry, photoluminescence (PL) measurements, and spectroelectrochemistry; however, the success in the determination of the redox properties as already reported has been low. We now describe a simple method for the determination of the redox potentials of many individual (n,m)SWNTs using near-IR PL spectroelectrochemistry.

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### Use of high energy spectroscopy to understand functionalized single-walled carbon nanotubes

**Paola Ayala**, *Universität Wien, Austria* | **Christian Kramberger**, *Universität Wien, Austria* | **Hidetsugu Shiozawa**, *University of Surrey, United Kingdom* | **Yasumitsu Miyata**, *Nagoya University, Japan* | **Hiromichi Kataura**, *AIST, Japan* | **Thomas Pichler**, *University of Surrey, United Kingdom*

Whether we are dealing with the inevitable interactions of nanotubes in a bundle or single doping defects, the energies of charge carriers and lattice vibrations are modified. For this reason, analysing the details in modifications of the underlying basic correlation effects in the bonding environments in a very effective manner is crucial. Our approach to this problem is mainly based on the use of techniques such as photoemission and x-ray absorption spectroscopy. I will show our recent progress on how metallicity-sorting combined with high energy spectroscopy techniques can nicely disentangle the characteristic density of states of SWCNTs unambiguously. A further insight into the influence of doping, chemical interactions on the electronic ground state and the transport properties of SWCNTs will be presented. We will analyze the changes in the site selective electronic structure within various types of metallicity pure SWCNTs (metallicity-sorted and functionalized), substitutionally doped nanotubes (with B and N), and filled with rare-earth.

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### Multiple in-situ field emission testing capabilities at GE Global Research

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For well-known reasons, carbon nanotubes (CNTs) are ideal candidates for field emission (FE). We have developed a modular and flexible FE testing system capable of accurately measuring currents from CNT devices as well as performing other in-situ characterization, including visualization of the emitted electron beam. Electrical testing of each sample includes multiple modes (DC, as well as single and repetitive pulses, each of 20 microsecond duration) between a parallel, translatable anode, with an applied electric field of up to 20 V/micron. A testing protocol that optimizes output electron emission current and lifetime was designed to address reliability and robustness of the CNT field emitters. This involves generating a continuous series of at least 100,000 pulses at increasing anode electrical potentials for each device. A set of CNT FE devices provided excellent average current density during lifetime testing (1 A/cm2) for several million cumulative pulses.

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### Roles of Acid Treatments on the Networks of Single-Walled Carbon Nanotube Devices

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Various chemical modifications of the side wall of single-walled carbon nanotubes (SWCNTs) have been used for various purposes such as separation, purification, doping, and functionalization of SWCNTs. Some of these chemicals directly and locally modify sp2 carbon bonds of SWCNTs, physisorb on the surface of SWCNTs, or intercalate into SWCNT-SWCNT junctions. As a result, these chemical treatments can change electronic structures of SWCNTs, thereby affects electrical transport characteristics of SWCNT-based devices. In this study, we investigate the effects of acid treatments on the electrical transport characteristics of SWCNT network devices. As-fabricated SWCNT network devices are exposed to nitric acid vapor at elevated temperature. IV characteristics of the devices before and after the exposure show mostly changes in the threshold voltages, overall current levels, and hysteresis. In addition, the reversibility or irreversibility of the changes is also investigated by removing acid molecules using vacuum annealing. In order to elucidate the roles and mechanisms of the acid treatments, local electrical properties of the devices during the whole processes are measured with electrostatic force microscopy and scanning gate microscopy. These local measurements reveal changes in the gate responses of the local parts of the devices and contact resistances at various parts of the devices such as SWCNT-SWCNT and SWCNT-electrode junctions. Correlations with the whole device operation characteristics will also be discussed.

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### Highly sensitive UV sensor using SWNT- ZnO heterojunctions

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Heterojunctions with various compositions and interfaces create built-in electric fields that deplete or accumulate electrons and holes within the nanostructure, which have already demonstrated distinctive performances in nanodevice applications for optoelectronic technologies like light-emitting diodes, photovoltaics, and optical sensors. There has been great interest in UV sensor based on single walled carbon nanotube (SWNT)-zinc oxide (ZnO) heterojunctions because SWNTs can enhance UV photoresponse. The SWNT-ZnO heterojunction film was fabricated by two step processes: first, a SWNT Langmuir-Blodgett (LB) film was deposited on an anodic aluminum oxide (AAO) template; and then, ZnO film was made by vacuum filtration of ZnO nanowire solution. The UV sensor based on combination of SWNT-ZnO demonstrated fast photoresponse. We also observed highly efficient photovoltaic effects in the SWNT-ZnO junctions when the device was illuminated by UV radiation. Furthermore, the mechanism of UV sensitivity enhancement and photovoltaic effects was assumed to result from the high electron mobility in the SWNT-ZnO heterojunctions.

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### Supramolecular Assembles of Carbon Nanohorns and Porphyrin for Photoinduced Electron Transfer System

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Carbon Nanohorns1 (CNHs) represent a new type of nanostructured carbon-based material. CNHs have attracted a great deal of attention in several fields as optoelectronic applications2. Combination of covalent and non-covalent functionalization of CNHs is particularly promising for building donor–acceptor nanohybrids. Among various non-covalent methodologies reported, self-assembly by using an ammonium ion-crown ether interaction is regarded as one of the most powerful methods. Porphyrin / Fullerene based donor–acceptor supramolecular systems involving crown ether-ammonium interactions have been prepared for probing photo-induced electron processes.3 This concept has been extended to build porphyrin / SWNT donor–acceptor nanohybrids, and occurrence of photo-induced charge separation processes is clearly demonstrated.3 Herein, we describe a supramolecular assemble of CNH covalently bonded with amino groups via spacer (sp) (CNH-sp-NH3+), which is included in crown-ether appending porphyrin (Crown-ZnP). Nanohybrid CNH-sp-NH3+ and the supramolecular assemble CNH-sp-NH3+;Crown-ZnP were characterized by means of several techniques as HR-TEM, TGA, XPS, Raman, FT-IR and UV-vis spectroscopies. Photoinduced electron-transfer processes of the nanohybrids are confirmed on combining the time-resolved absorption and fluorescence measurements, in addition to the accumulation of viologen cation radical in solution with steady-light illumination. The efficiency of this system in photovoltaic solar cells is shown. (1). Iijima, S.; Yudasaka, M.; Yamada, R.; Bandow, S.; Suenaga, K.; Kokai, F.; Takahashi, K. Chem. Phys. Lett. 1999, 309, 165. (2) Sandanayaka, A. S. D.; Ito, O.; Tanaka, T.; Isobe, H.; Nakamura, E.; Yudasaka, M.; Iijima. S. New J. Chem. 2009, 33, 2261. (3) D'Souza, F.; Ito, O. Chem. Commun. 2009, 4913.

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### Polymer and Protein Adsorbed Phases for Near-Infrared Fluorescent Detection of Glucose Using Single-Walled Carbon Nanotubes

**Michael Strano**, Massachusetts Institute of Technology | **Hyeonseok Yoon**, *Massachusetts Institute of Technology* | **Paul Barone**, *Massachusetts Institute of Technology* | **Jin-Ho Ahn**, *Massachusetts Institute of Technology*

This presentation describes novel approaches to glucose detection using single-walled carbon nanotube (SWNT)-based optical sensors. The functionalization of SWNT is of key importance for applications in optoelectronics, biological imaging, and sensing. Here, SWNT is suspended with appropriate polymers in aqueous solution and then further functionalized with receptor proteins. For example, poly(vinyl alcohol) (PVA)/SWNT hydrogels are made to demonstrate the use of hydrogel swelling as a mechanism to reversibly induce solvatochromic shifting in SWNT near-infrared emission. The optical sensor reports the degree of the glucose concentration when a glucose receptor is used to cross-link the hydrogel. PVA/SWNT hydrogels are initially made via dialysis of PVA/SWNT solution, followed by cross-linking reaction. The hydrogels are further modified to incorporate carboxyl groups and glucose binding receptors were covalently attached to PVA hydrogel matrices. Several glucose binding receptors are tested for efficacy within the PVA hydrogel system, eventually settling on apo-glucose oxidase as a means to reversibility and stably modulating the dielectric environment in response to glucose. The change in the dielectric environment affects strongly the SWNT fluorescence, which allows rapid and reversible glucose recognition. This is the first demonstration of a glucose receptor as a selective binding site to modify the dielectric environment in this type of material. SWNT fluoresce in the near infrared where human tissue penetration is maximum and biological autofluorescence is minimal. In addition, the polymer PVA is biocompatible. Therefore, these new platforms have high potentials toward tissue implantable sensors.

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### Resonant Raman Spectroscopy of Semiconducting Single Walled Carbon Nanotubes

**Juan Duque**, *Los Alamos National Laboratory* | **Hang Chen**, *Boston University* | **Anna Swan**, *Boston University* | **Ming Zheng**, *National Institute of Standards and Technology* | **Stephen K. Doorn**, *Los Alamos National Laboratory*

Recent advances in carbon nanotube separations science are providing access to samples highly enriched in single chiralities. We present a Raman spectroscopic investigation of enriched semiconducting samples. Resonance Raman excitation profile between 1.75 and 2.25 eV (E22 transition) and between 3.1 and 3.5 eV (E33 and E44 transitions) of RBM, G-band, and G' spectra from isolated SWNT samples will be presented. RBM profiles show very good separation of single chirality semiconducting fractions with very low cross-contamination from other nanotubes. G-band profiles allow testing of different models for the Raman scattering process and reveal new evidence for the importance of non-Condon and interference effect in the Raman response. Investigations into the behavior of the highly dispersive G' mode enabled us to map the band structure of the different isolated chiralities and to probe variable coupling in the vicinity of the E22 transition. These results demonstrate the important role that chirality-enriched samples have to play in revealing new SWNT photophysical.

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### Raman Spectroscopy and Low-Temperature Transport Measurements of Individual Single-Walled Carbon Nanotubes With Varying Thickness

**Jyri Rintala**, *Nanoscience Center, Department of Chemistry, University of Jyväskylä, Finland* | **Olli Herranen**, *Nanoscience Center, Department of Physics, University of Jyväskylä, Finland* | **Andreas**

**Johansson**, *Nanoscience Center, Department of Physics, University of Jyväskylä, Finland* | **Markus Ahlskog**, *Nanoscience Center, Department of Physics, University of Jyväskylä, Finland* | **Mika Pettersson**, *Nanoscience Center, Department of Chemistry, University of Jyväskylä, Finland*

We have investigated [1] two metallic and one semiconducting individual single-walled carbon nanotubes (SWCNT) and one bundle of two semiconducting nanotubes with a diameter range of 1.1-2.9 nm with Raman spectroscopy and low-temperature electrical transport measurements. With these two methods, we obtain mutually independent measurements on the basic properties of a specific nanotube. In particular, we obtain data on metallic and semiconducting properties. Evidence of a small band gap for one metallic tube was obtained. For the semiconducting SWCNTs with diameters of 2.7-2.9 nm, a special resonance condition was observed which causes an anomalous intensity ratio for the two components of the G-band. This effect has been observed [2] previously for a few tubes with diameter of 1.6 nm, and our current findings are in agreement with the previously given explanation of the effect and suggest that the effect is common among thick SWCNTs. We also obtain evidence that the currently used relations between the frequency of the radial breathing mode and tube diameter tend to underestimate the diameter for thick tubes. References [1] J. Rintala, et al., J. Phys. Chem. C 113, 15398 (2009). [2] A. Jorio, et al., Phys. Rev. B 65, 155412 (2002).

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### Curvature Effects on Optical Transitions in Semiconducting Carbon Nanotubes with Small Diameters

**Saloome Motavas**, *Department of Electrical and Computer Engineering, University of British Columbia* | **Andre Ivanov**, *Department of Electrical and Computer Engineering, University of British Columbia* | **Alireza Nojeh**, *Department of Electrical and Computer Engineering, University of British Columbia*

Due to their unique physical and electronic properties, carbon nanotubes are attractive candidates for optoelectronic and nanophotonic applications. Curvature and rehybridization strongly affect the electronic structure of small-diameter nanotubes and, as a consequence, have important implications on their optical properties. Here, we use first-principles/density functional theory calculations to study the curvature effects on the optical transitions in a number of semiconducting zigzag nanotubes with progressively smaller diameters, down to (4,0) nanotubes. We investigate the optical transition dipole moments and absorption rates for all possible transitions between various pi and sigma bands (including pi-sigma transitions) and the corresponding selection rules. We also examine how curvature affects the polarization dependence of light absorption. Various polarization angles ranging from parallel to perpendicular to the nanotube axis are considered. In general, for transitions from each valence sub-band, we observe that the parallel component of the dipole is a few times to an order of magnitude larger than that of the perpendicular component. Some exceptions exist; however, these usually correspond to large photon energies, leading to a low corresponding transition rate. For example, for an (8,0) nanotube, we show that the overall transition rate spectrum for perpendicular-polarized light is suppressed noticeably compared to the one for the parallel polarization of light. The relative strength of the parallel component of the dipole moment becomes stronger as the nanotube diameter decreases. To further investigate the curvature effects, we compare the results with those predicted using the conventional, pi-orbital tight-binding calculations within the zone-folding scheme.

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### Anisotropic Electro-optical Effects in Aligned Single-Walled Carbon Nanotubes

**Eri Maruyama**, *Graduate School of Information Science and Technology, Hokkaido University* | **Kenji Yamamoto**, *Graduate School of Information Science and Technology, Hokkaido University* | **Agus Subagyo**, *Graduate School of Information Science and Technology, Hokkaido University* | **Cary L. Pint**, *Department of Chemistry, Rice University* | **Robert H. Hauge**, *Department of Chemistry, Rice University* | **Junichiro Kono**, *Department of Electrical and Computer Engineering, Rice University* | **Kazuhisa Sueoka**, *Graduate School of Information Science and Technology, Hokkaido University*

Strong electric fields are expected to induce non-trivial modifications to the optical properties of single-walled carbon nanotubes (SWNTs). Depending on the field direction and strength, a variety of electro-optical (EO) phenomena are predicted: the quantum-confined Stark effect, the Franz-Keldysh effect, and Stark shifts and ionization of excitons. In a parallel field in the strongest field regime, the Franz-Keldysh effect is expected to cause spectral oscillations (absorption) above (below) the band gap. Several groups have reported observations of EO modulations in SWNTs. However, configurations were not well defined in these experiments. Here, we have fabricated a novel EO device in which the directions of the electric field, nanotube axis, and light polarization were very well defined. We used highly-aligned, CVD-grown SWNTs in combination with interdigitated electrodes. We observed field-induced transmission changes only when the field was parallel to the tube axis, and the largest change was observed when the polarization was also parallel to the tube axis. With fields up to 40 kV/cm, we were able to induce transmission changes of <8E-3. The effect was also strongly dependent on the photon energy. At energies >0.8 eV, the transmission change exhibited a quadratic dependence on the field, indicative of a Stark effect. In conclusion, we observed anisotropic EO effects in SWNTs for the first time. This was achieved by using highly-aligned SWNTs combined with a well-defined electrode structure. Large EO signals were obtained only when both the light polarization and electric field were parallel to the nanotube axis.

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### Exploring and Enhancing the Fluorescence Quantum Yield of Single-Walled Carbon Nanotubes

**Nicole Briglio**, *University Of Rochester Department of Chemistry* | **Julie Smyder**, *University Of Rochester Department of Chemistry* | **Lisa Carlson**, *University Of Rochester Department of Chemistry* | **Kathryn Leach**, *University Of Rochester Department of Chemistry* | **Andrea Lee**, *University Of Rochester Department of Chemistry* | **Xiaoyong Wang**, *University Of Rochester Department of Chemistry* | **Todd Krauss**, *University Of Rochester Department of Chemistry; University of Rochester Institute of Optics*

The quantum yield (QY) of ensemble samples of single-walled carbon nanotube (SWNT) suspensions is commonly measured to be less than 0.1%, but single molecule studies show that individual SWNTs have a photoluminescence QY of ~1%. Through the use of patterned substrates, we precisely and directly correlated the fluorescence from individual DNA-wrapped SWNTs with atomic force microscopy (AFM) topography images of the same SWNTs. By employing this method, we can demonstrate that the poor QY of SWNTs arises from only a small population (~6%) of bright emitters while the rest of the nanotubes are quenched. Due to recent observations of fluorescence quenching in DNA wrapped SWNTs, we are currently exploring the use of non-natural peptides as wrapping agents. Biocompatible peptide structures can be tailored to exhibit certain properties, which may increase interactions with SWNTs of specific chiralities. We have also consistently observed enormous enhancement of the QY for individual SWNTs to unprecedented values of ~30% resulting from the addition of reducing agents to aqueous SWNT solutions. These unexpectedly high QY values indicate that SWNTs are intrinsically bright emitters, and that current understanding of the optical properties of SWNTs has largely been obtained from defective SWNTs having photoluminescence partially quenched. The availability of a bright and steady source of NIR photons will greatly facilitate the development of the new technology in several fields including biological imaging, quantum optics, and optoelectronics.

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### Photoluminescence saturation at low exciton densities in single air-suspended SWNTs indicating new microscopic exciton interaction mechanisms

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Under low optical excitation fluences (quasi-uniform excitation, polarized parallel to tube axis, resonant to E22), single air-suspended single-walled carbon nanotubes (SWNTs) with minimal environmental perturbations exhibit high photoluminescence (PL) action cross sections (0.5-3.5x10^-18 cm2/atom), high PL quantum efficiencies (7- 20%) and narrow emission linewidths (~12 meV) at E11[1]. At a moderate excitation fluence (<10^12 photons/cm2/pulse), PL emission saturates drastically and does not increase further as the excitation fluence is raised tenfold. A stochastic model is adapted [2] to fit experimental results with both excitation and emission fluence of single SWNTs presented in true units. The results show that the onset of PL clamping corresponds to the injected exciton number 2 – 6 in the micron-long SWNTs. Such extreme PL saturation at moderate excitation fluences cannot be explained by the commonly accepted diffusion-limited exciton-exciton annihilation model with diffusion lengths 6-90 nm[3] for surfactant encapsulated SWNTs. To further understand the efficient exciton-exciton interactions at low exciton densities in pristine single air-suspended SWNTs, we are currently studying the temperature and SWNT length dependence of PL saturation, specifically of the emission in saturation and the excitation fluence at the onset of PL saturation. The results will help to clarify the microscopic exciton interaction mechanisms in a quasi-1D system. References 1. Y.-F. Xiao et al. Phys. Rev. Lett. 104, 017401 (2010) 2. A. V. Barzykin and M. Tachiya, Phys. Rev. B 72, 075425 (2005). 3. Y. Murakami and J. Kono, Phys. Rev. Lett. 102, 037401 (2009).

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### Torsional Instability of Chiral Carbon nanotubes investigated

**Eduardo Barros**, *Universidade Federal Do Ceará* | **Daniel G. Vercosa**, *Universidade Federal Do Ceará* | **Georgy G. Samsonidze**, *University of California at Berkeley* | **Antonio G. Souza Filho**, *Universidade Federal Do Ceará* | **Riichiro Saito**, *Tohoku University* | **Mildred S. Dresselhaus**, *Massachusetts Institute of Technology*

Several theoretical and experimental studies indicate that the electronic and optical properties of carbon nanotubes are extremely sensitive to structural deformations such as axial, radial or torsional strains. However, these reports assume that in its natural state, carbon nanotubes are free from such geometrical deformations. As discussed in a recent publication, this is not the case for small diameter chiral carbon nanotubes, for which the presence of a torsional instability gives rise to a natural torsion. [1] The dependence of the magnitude of the natural torsion on the nanotube diameter and chiral angle was shown to be different for metallic and semiconducting nanotubes. The fact that chiral nanotubes are naturally torsioned has important implications on its fundamental physical properties. In this work, we use an extended tight-binding (ETB) approach [5], with a DFT calculation-based parameterization, in order to calculate the effects of the natural torsion to the optical and electronic properties of single-wall carbon nanotubes. The optical transition energies of the naturally torsioned semiconducting nanotubes were found to be shifted by as much as 64 meV when compared to that of their untorsioned structure and this difference was found to decrease as the inverse cube of the nanotube diameter. Also, the presence of a natural torsion causes an increase the "minigap" metallic tubes of up to 65%. Also, the physical origins of this instability and of its effects are discussed in detail. [1] Vercosa et al. Phys. Rev. B to be published (2010).

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### The Four-Level Model for the Raman Excitation Profile of Carbon Nanotubes

**Hang Chen**, *Boston University* | **Andy Walsh**, *Boston University* | **Juan Duque**, *Los Alamos National Laboratory* | **Stephen Doorn**, *Los Alamos National Laboratory* | **Anna Swan**, *Boston University*

Resonance Raman spectroscopy (RRS) has proven to be an efficient technique in the determination of the optical transition energies of carbon nanotubes (CNTs). The resonance Raman excitation profile (REP) obtained from RRS displays the Raman intensity from the CNT versus the laser energy, showing both the incoming and outgoing resonances, and can be utilized to investigate the electronic transition and vibration energies of the CNTs. Albeit several models have been formulated in the past to describe the REP with a symmetric lineshape, our experimental data for the E22 transition energy of G band and RBM spectra of various chiralities show a high asymmetry in the REP, indicating the inadequacy of the previous models. Here, we introduce a four-level model for the CNT REP derived via a third order, perturbative density matrix approach, allowing for the non-Condon effect. In this approach, the wave mixing energy level (WMEL) diagram is applied to a four level system (representing the ground and excited electronic state, each with zero or one phonon) of CNT to describe the time evolution of the system at the amplitude level. Advantages and limitations of the four-level model will be discussed by comparing it with other models.

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### Dynamic Alignment of Single-Walled Carbon Nanotubes in Pulsed Magnetic Fields

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The dynamic alignment allows the investigation of 2 fundamental physical properties of carbon nanotubes, i.e. the magnetic susceptibility through the total amount of aligned tubes in a liquid suspension and the dynamic behaviour of this tubes treated as rodlike particles. Semiconducting tubes are diamagnetic both along and perpendicular to their long axis but the magnitude of the perpendicular susceptibility is higher. Metallic tubes are paramagnetic along their long axis and diamagnetic perpendicular to it. This constrains SWNT to align parallel to a magnetic field. The brownian motion is the competing force against the external field and cause isotropic alignment in its absence.

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### Pi-stacking functionalization of single wall carbon nanotubes: Synthesis of complexes for energy transfer

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Chemical functionalization of carbon nanotubes is one of the key challenges towards their use in opto-electronic devices. This technique aims at combining the great transport properties of nanotubes with the versatility of the optical properties of organic molecules. An organic molecule acting as an antenna, coupled to a nanotube acting as a collector is an important step forward for applications in photovoltaic devices. We report on a synthesis protocol for the realization of controlled, reproducible and stable suspensions of single wall carbon nanotubes/porphyrin molecules complexes. These complexes present an efficient energy transfer from the molecules to the nanotube [1,2]. The starting material is an aqueous suspension of individual nanotubes in micelles and the functionalization is achieved by "Pi-stacking". The analysis of the functionalization process reveals the key role of the organic solvent of porphyrin molecules. The stability and the functionalization degree of the solutions are tracked by optical absorption. The amplitude of the Soret band of the stacked porphyrin molecules and the red-shifted S11 bands of the nanotubes are two reliable signatures of functionalization degree of the nanotubes. We describe the optimal synthesis conditions to realize a full coverage of the nanotube wall by porphyrin molecules [3]. The energy transfer occurring in these complexes is characterized by photoluminescence excitation measurements.  [1] G. Magadur et al. ChemPhysChem 2008, 9, 1250. [2] J.P. Casey et al. J. Mat. Chem. 2008, 18, 1510. [3] C. Roquelet, et al. arXiv 2009, 0910.5619v1.

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### Highly effective purification of carbon nanotubes by plasma-thermal annealing

**Reinhard Mach**, *BAM - Federal Institute for Materials Reseach and Testing* | **Heinz-Eberhard Maneck**, *BAM - Federal Institute for Materials Reseach and Testing* | **Franz Oleszak**, *BAM - Federal Institute for Materials Reseach and Testing* | **Asmus Meyer-Plath**, *BAM - Federal Institute for Materials Reseach and Testing*

A new, very rapid and highly effective method has been developed for the gas-phase purification of CNT. CNT were injected into a thermal atmospheric plasma jet of about 10000 K enthalpy. A single passage of a few milliseconds duration was found to significantly reduce catalyst metal, metal oxides, and functional impurities. For unpurified commercial multi-walled CNT from CVD with an ash content of 1.8 wt.% and 20 wt.% the ash content was reduced to 0.2 wt.% and 4 wt.%, respectively. Also the concentration of hydrogen and oxygen impurities was found to decrease. CNT impurities were quantified by ICP-MS, ashing in air at 800 °C, TGA, and elemental analysis. Investigations by SEM and TEM showed that the nanoscopic CNT structure remains intact. Raman and XRD measurements indicate structure improvements. For several CNT samples, an impressive increase of the oxidation resistance of more than 120 K was observed by TGA. Results of systematic studies on the process purification efficiency will be reported in dependence on the plasma power, mass feed rate, and processing gas composition for different types of CNT. They show that the new method is a highly promising alternative to traditional acid treatment of CNT or high-temperature annealing in a furnace.

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### Electrochemical Oxidation Behavior in Single-Wall Carbon Nanotubes

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For developing application of single-wall carbon nanotubes (SWCNTs), the length is one of the most important structural parameters, since it affects on their dispersibility and processability, as well. Many researchers have been reported cutting processes of SWCNTs, however, it still quite difficult because of their robustness. In this study, we have investigated the cutting method via electrochemical oxidation of SWCNTs in pure water with applying direct current (DC) voltage. SWCNTs with ca. 0.9 nm diameter, synthesized by the enhanced direct-injection pyrolytic-synthesis (e-DIPS) method were used in this study. The working electrode fabricated by SWCNTs sheet and a counter platinum electrode were settled in the vessel filled with Mili-Q water (Millipore) separately, and then DC voltage was applied between the electrodes for 10 hours. After the voltage of +4 V was applied on SWCNTs electrode, a considerable amount of shortened SWCNTs with 1 nm diameter were observed by transmission electron microscopy (TEM). When applied voltage was increased to +10 V, SWCNTs observed to be completely collapsed into amorphous carbon, although rarely found to be remained wide SWCNTs (>2nm), which also observed in the starting material. In conclusion, the cutting of SWCNTs was observed with around +4 V voltage. It also suggests that the diameter selective cutting of SWCNTs could be provided with controlling the applied DC voltage.
Acknowledgment This work has been supported by New Energy and Industrial Technology Development Organization (NEDO) project.

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### Microwave-assisted bromination of double-walled carbon nanotubes

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The ability to functionalize carbon nanotubes (CNTs) through controlled structural modifications is an essential prerequisite for application purposes. A major challenge in this field, therefore, is to develop a range of reliable and effective functionalization methodologies that allow the design of CNTs-based macromolecular species of highly versatility and usefulness. Moreover, the modifications of CNTs do not extensively disrupt the graphitic p-conjugated surface, and consequently do not alter their electronic and optical properties. In this respect, halogenated CNTs-based materials can represent an useful class of intermediates as they are precursors to a number of interesting reactions. Here, we report on the synthesis and characterization of double-walled carbon nanotubes (DWCNTs) functionalized with Br2 under microwave-assisted conditions. Comprehensive characterization of the functionalized carbon networks shows that the Br atoms are covalently linked to DWCNTs, with a percentage of functionalization of ca. 5-8% in weight as determined from X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray (EDX), and thermogravimetric analysis (TGA) experiments. These new modified CNTs-based precursors could open new synthetic possibilities for designing novel functionalized CNTs using metal-catalyzed cross-coupling reactions, further expanding the versatility and applications fields of this fascinating allotropic family of carbon.

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### Nitrogen-doped carbon nanotubes as a highly active metal-free catalyst for selective oxidation

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The introduction of dopant atoms, i.e. nitrogen and/or boron, inside the 1D carbon material leads to a new class of material with improved catalytic performance. Recent reports have revealed the fact that nitrogen-doped carbon nanotubes (N-CNTs) can be efficiently employed as catalyst for the Oxygen Reduction Reaction

(ORR). According to these results one can expect that N- CNTs can be efficiently used as a metal-free catalyst for other oxidative reactions in place of the traditional supported metal catalysts. Here we report for the first time the use of the N-CNTs as a metal-free catalyst for a selective oxidation reaction to convert a harmful species like $H_2S$ into elemental sulfur. The N-CNTs were synthesized by a chemical vapor deposition (CVD) method using a mixture of $C_2H_6$, Ar and $NH_3$ over $Fe/Al_2O_3$ catalyst. The as-synthesized material was treated with a base (NaOH) and acid (aqua regia) at 110°C for 24h in order to remove the residual iron and alumina. XPS analysis done on the N-CNTs shows 2 at.% nitrogen doping in these N-CNTs and less than 0.1 at.% of iron residue after their purification by acid treatment. These metal-free catalysts exhibit an extremely high desulfurization activity compared to the traditional iron-based catalysts ($Fe_2O_3$/CNT and $Fe_2O_3$/SiC with 3 wt.% of Fe) under industrial reaction conditions. It is noteworthy to indicate that undoped CNTs show no catalytic activity for this reaction. N-CNTs also exhibit an extremely high stability as no catalytic change was observed for a time period of more than 100 hours.

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### Synthesis and characterization of cyano functionalized SWCNT

**Kemei Cheng**, *Institute Of Chemical Materials* | **Zhong Wei** | **Liang Du** | **Junqing Yang**, *Department of material science and engineering*

For the first time, cyano modified single walled nanotube (CN-SWCNT) was synthesized and characterized in our group. After the synthesis, we investigated the effect of cyano group on the electronic performance of single walled nanotube (SWCNT) with UV-vis spectrum. SWCNT was sythesized using CVD method. The CN-SWCNT was synthesized by three steps. amorphous carbon was removed using nitric acid and sulfuric acid mixture (volume ratio= 1:3) in sonication. Then SOCl-SWCNT was prepared according to method in other papers]. A. Hulkengerg's paper was used as reference in our experiments as no public synthesis method for the synthesis of CN-SWCNT. This paper was about how to tranfering acid chlorides i nto nitriles by one pot synthesis method. The typical procedure of our synthesis was: 0.01 mole of SOCl-SWCNT and 0.012 mole of sulfonamide are dissolved in 10 ml of sulfolane and the solution is subsequently warmed for six hours at 12OoC. After cooling, the reaction mixture is poured into 150 ml of 1 N sodium hydroxide and filtered using PTFE film. The solid was then washed three times with water in order to remove traces of sulfolane. The product was dryed in an oven for one day. The product was verified using IR, XPS and Raman spectrum. At last, the electroic performance of CN-SWCNT was characterized using UV-vis spectrum, and compared with that of the original SWCNT.

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### Control of covalent functionalization for designing new CNT based materials

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Carbon nanotubes (CNTs) are described since several years as the material of the future. Several limitations make them difficult to use, in particular their poor solubility and virtual chemical inertness. Covalent functionalization of CNTs has been used extensively to solubilize or disperse and therefore manipulate these exceptional materials. It may also be helpful to give the CNTs additional physical and/or optical properties, such as possible photo-induced electron transfer, through the grafting of functional groups. However covalent derivatization alters the electronic system of CNTs and thus their properties, and attempts should be made to limit its extent. Although many reported functionalization routes are known,[1] most involving highly reactive intermediates, the functionalized ratio is not controlled. An original way of functionalization has been developed in our laboratory: CNTs are functionalized through their reduction into salts. It enables to obtain a control of the functionalization ratio [2]. We have applied the new method to graft original chemical groups such as organic dyes or modified mesogen molecules. Results obtained from these new materials with various extents of functionalization will be exposed.

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### In situ Purity Enhancement and Surface Modification of Single-Walled Carbon Nanotubes Synthesized by Induction Thermal Plasma

**Ali Shahverdi**, *Université de Sherbrooke* | **Keun Su Kim**, *Université de Sherbrooke* | **Yasaman Alinejad**, *Université de Sherbrooke* | **Sanaz Arabzadeh**, *University of Toronto* | **Javad Mostaghimi**, *University of Toronto* | **Gervais Soucy**, *Université de Sherbrooke*

A facile, inexpensive, and energy efficient process was developed for the in situ purification and surface modification of Single-Walled Carbon Nanotubes (SWCNTs) produced by the induction thermal plasma process. The SWCNT materials were thermally treated with an oxygen flow in synthesis system while they are assembled into SWCNT sheets. According to the results, the amount of amorphous carbon impurities in the final product was considerably reduced due to the selective oxidation of amorphous carbon at high temperatures (i.e., 593 K). Three different flow rates of oxygen were tested and the results clearly confirmed a complete removal of amorphous carbon from the SWCNTs product at an oxygen content of 10 vol. % (i.e., 17.22 SLPM) in the synthesis system. Moreover, it has been found from the surface characterization studies by XPS that this in situ thermal oxidation process also modified the surfaces of the SWCNTs with oxygen functional groups.

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### Cycloaddition of benzyne to SWCNT. Towards carbon nanotube-based gears (paddle-wheels)

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Carbon nanotubes have many attractive material properties. For example, experiment and theory have demonstrated that nanotubes have exceptionally high Young's modulus and nanotube electronic properties vary as a function of diameter and chirality. These properties have opened doors to electronic, optical, magnetic and mechanical applications. In addition, the functionalization of carbon nanotubes provides opportunities for fabrication of novel nanodevices. In this respect, it have been suggested that it may be possible to make nanotube based molecular gears by bonding rigid molecules onto nanotubes to form gears with molecular teeth. Herein, we report the functionalization of SWNTs using benzyne generated by different methods. Full characterization of cycloadducts has been performed by means of several techniques: Raman spectroscopy, TGA, HR-TEM, XPS, UV-vis-NIR and FTIR. Determination of the diameter of carbon nanotube allowed us to distinguish between the two types of products that can be formed by reaction of carbon nanotubes and benzyne, the 1,2 and 1,4 adducts.

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### Multi-walled carbon nanotubes functionalized with silver nanoparticles

**Fernando Monteiro**, *Pontificia Universidade Catolica Do Rio De Janeiro* | **Dunieskys Larrudé**, *Pontificia Universidade Catolica Do Rio De Janeiro* | **Marcelo Maia Costa**, *Pontificia Universidade Catolica Do Rio De Janeiro* | **Fernando Freire Jr.**, *Pontificia Universidade Catolica Do Rio De Janeiro* | **Erik Talarico**, *Pontificia Universidade Catolica Do Rio De Janeiro*

In recent years, many efforts have led to the development of versatile methods to modify carbon nanotubes (CNTs) to obtain derivatives with more attractive features. To this end, CNTs decorated with metal nanoparticles (NPs), which exhibit increased chemical activity due to their large surface to volume ratios and crystallographic surface structure, have been examined toward applications in the area of nanoelectronics, as gas sensors and in heterogeneous catalysis. In this work, multi-walled carbon nanotubes (MWCNTs) have been synthesized by the Spray Pyrolysis method using toluene and ferrocene as precursors. After that, a stable homogenous MWCNTs suspension was obtained by dispersing 25mg of pristine MWCNTs into 1.0wt% of sodium dodecyl sulfate (SDS) aqueous solution and sonicated for two hours. The resultant MWCNTs suspension was introduced to the Tollens reagent formed adding to a 1.0wt% of silver nitrate (AgNO3) solution 5% of ammonia drop wise under stirring until the brown precipitate just dissolved. Formaldehyde (0.5ml) were dropped to the system and the system was kept stirring at 60C for 45min. The silver-functionalized MWCNTs were collected by centrifugation and washed with water and ethanol several times. The obtained black powder was dried at room temperature for 24 hours. Different concentration of silver nitrate solutions were used varying from 0.2 to 1.0wt %.The surface analysis was carried out using electron microscopy, both SEM and TEM, and shows silver nanoparticles uniformly dispersed around the CNTs surface with NPs diameters smaller than 50nm. Raman and XPS were also performed to characterize the functionalized MWCNTs.

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### Different chemical approaches to the modulation of CNT properties

**Enzo Menna**, *ITM-CNR and Università Di Padova*

We report about the study of different strategies for the functionalization of carbon nanotubes (CNT) that, tanks to their unique dimensionality and structure, could lead to the development of new functional nanomaterials with peculiar properties potentially useful in different application fields. The first approach is based on the covalent functionalization of single wall carbon nanotubes (SWNT) with poly(ethylene glycol) chains (PEG), and the co-functionalization with PEG and different polycyclic aromatic fluorophores. [1, 2, 3] Such derivatives, soluble both in water and organic solvents, have been fully characterized with a special focus on the photophysical properties: electronic interactions between nanotube and fluorophore, have been highlighted. The second strategy consists of the encapsulation, of different types of organic molecules (fullerene derivatives and polycyclic aromatic molecules) inside the inner space of the SWNT. Results obtained from the different encapsulating procedures have been compared.[3, 4] The third functionalization approach involves non-covalent interactions between the exterior walls of the CNT and proper molecules (such as bis-styrilbenzene derivatives) to allow a fast and efficient dispersion in organic solvents. Through casting over glass substrates, nanostructured coatings have been obtained with peculiar wetting behaviors.  References 1. M. D'Este, M. De Nardi, E. Menna; Eur. J. Org. Chem. 2006, 2517-2522. 2. A. Gambetta, C. Manzoni, E. Menna, et al.; Nature Phys. 2006, 2, 515-520. 3. F. Cordella, M. De Nardi, E. Menna, et al. Carbon 2009, 47, 1264-1269 4. M. A. Loi, J. Gao, F. Cordella, P. Blondeau, E. Menna, et al.; Adv. Mater. (DOI: 10.1002/adma.200903527)

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### Elaboration and properties of hybrid carbon nanotubes – Pi conjugated molecules

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Hybrid nanostructures based on carbon nanotubes functionalized with Pi-conjugated molecules are excellent candidates to build high performance functional optoelectronic and sensor devices. [1] In this approach, the grafted molecules act as an antenna and the NT as a collector. The aims are to combine the remarkable transport properties and sensitivity of NTs with the versatility of the optical properties of organic molecules or with the ultimate selectivity of chemical or biological receptors. Several issues have to be addressed to make this approach viable: e.g., the NT and grafted molecule properties have to be preserved; the information transduction has to be enabled and efficient. We used different chemical routes (diazonium, organometallic coupling, (2,1) addition) [1] to graft conjugated oligomers (diphenylacetylene) on NTs and investigated the resulting hybrid system by resonant Raman spectroscopy, XPS, optical absorption and photoluminescence. The estimate of the number of addends per carbon atom from XPS and Raman spectroscopy [2] (D band of the NTs and triple bound band of the diphenylacetylene) will be presented. The impact of functionalization on the NT properties will also be discussed and the different chemical reactions used will be compared. [1] X. Peng, S.S. Wong, Advanced Materials 21, 625 (2009); S. Banerjee et al., Advanced Materials 17, 17 (2005); A. Hirsch, Ang. Chem. Int. Ed. 41, 1853 (2002); YL Zhao et al., Acc. Chem. Res. 42, 1161 (2009). [2] C. Fantini et al., J. Phys. Chem. C 111, 17941 (2007); C. Fantini et al., J. Phys. Chem. C 112, 13150 (2008).

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### Functionalization of Multilayer Fullerenes (Carbon Nano-Onions)

**Kevin Flavin**, *Trinity College Dublin* | **Manuel Chaur**, *Clemson University* | **Luis Echegoyen**, *Clemson University* | **Silvia Giordani**, *Trinity College Dublin*

Multishell fullerenes, also known as carbon nano-onions (CNOs) display several very unique properties, such as a large surface area to volume ratio, a low density and a graphitic multilayer morphology, which makes them appealing for many potential applications, such as catalysis, gas storage, electromagnetic shielding, and optical limiting. We have developed a novel versatile approach for the functionalisation of CNOs which allows us to introduce of a variety of functionalities onto their surface by treatment with in-situ generated diazonium compounds, complemented by use of "click" chemistry. We used Thermogravimetric Analysis, Raman Spectroscopy, UV-vis-NIR Absorption Spectroscopy, FTIR and Emission Spectroscopy to fully characterize the functionalised carbon nano-onions.   Reference: Flavin K., Chaur N., Echegoyen L. and Giordani S. "Functionalisation of multilayer fullerenes (carbon nano-onions) using diazonium compounds and 'Click chemistry'" Org. Lett. 2010, 12, 840-843.

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### Stable suspensions of Fe-filled carbon nanotubes for potential biomedical applications

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Biocompatible ferromagnetic Fe-filled carbon nanotubes (Fe-CNTs) with tailored functionalities are foreseen as a promising tool for investigation of biological materials (cell, tissue, human body). Fe-CNTs, with a high aspect ratio and preferred magnetization direction along the axis, show a highly non linear anisotropic and hysteretic magnetization curve. The unique properties of Fe-CNTs open a perspective of entirely new detection techniques in biomedical applications, such as minimal-invasive interventions. These applications require individually dispersed Fe-CNTs in stable suspensions. In general, stability of magnetic particle suspensions results from the equilibrium between attractive (Van der Waals and magnetic dipolar forces) and repulsive forces. The latter are electrostatic and steric repulsions, as described by the DLVO (Derjaguin-Landau-Verwey-Overbeek) theory. In our study, Fe-filled multiwalled carbon nanotubes (Fe-MWNTs) are functionalized via the non covalent approach using a range of biocompatible dispersants (CMC-Na salt, Polylysine (Lys:Phe, 1:1) and PL-PEG-NH2). The relative stability of Fe-MWNTs using the different dispersants is demonstrated over a significant period of time by quantitatively analyzing the settling of Fe-MWNTs and the diffusion potential (æ-potential) related to the different dispersants. Furthermore, the effect of salt concentration and pH on stability and precipitation of the suspensions is analyzed. Finally, Fe-MWNTs colloidal suspensions are characterized with a vibrating sample magnetometer (VSM). Furthermore, thanks to the permanent magnetic dipole moment with a component along the axis of the Fe-MWNTs rotational motion of individual Fe-MWNTs is shown from complex magnetic susceptibility measurements.

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### Nitrogen-doped Carbon nanotube synthesize according to gas flow rate by Chemical Vapor Deposition

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Nitrogen-doped (N-doped) Carbon nanotubes (CNTs) have been prepared by Chemical Vapor Deposition (CVD). CVD is a normal technique to produce carbon materials. As doping accompanies with the recombination of carbon atoms into CNTs in the CVD process, N atoms can be substitutionally doped into the CNTs lattice, which is hard to realize by other synthetic methods. Doping of CNTs by boron and nitrogen renders them p-type and n-type, respectively. N-doped CNTs show n-type behavior regardless of tube chirality. The N-doped nanotubes show the G-band in the Raman spectrum at a lower frequency than the undoped ones. N doping introduces large amount of topological defects. Among all the doped CNTs, the N-doped CNTs are of special interest in both fundamental and application studies. We studied the growth of N-doped CNT with NH3 gas ratio in CVD. By using Raman and XPS, we demonstrate the existence of the N-doped CNT.

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### Characterization of carbon nanotube thin film transistors by scanning probe microscopy

**Yuki Okigawa**, *Nagoya University* | **Yutaka Ohno**, *Nagoya University* | **Shigeru Kishimoto**, *Nagoya University; VBL Nagoya University* | **Takashi Mizutani**, *Nagoya University*

Carbon nanotube thin film transistors (CNT-TFTs) are expected to be suitable for flexible and high-speed electronics [1]. In this study, we studied electrical properties of CNT-TFT channel using Kelvin probe force microscopy (KFM) [2], point-contact current-imaging AFM (PCI-AFM) [3], and scanning gate microscopy (SGM) [4]. The CNT-TFTs were fabricated using CNT networks directly grown on a SiO2/Si substrate by plasma-enhanced chemical vapor deposition [5]. The potential image obtained by KFM showed a terrace-like structure at Vds = -2 V and Vgs = 0 V. The boundaries of the terrace are rather parallel to the edge of the source and drain electrodes. In addition, it seems that the potential in each terrace is almost constant.
It is interesting to note that such a unique potential image was obtained even for the randomly-grown CNT network. In order to clarify the origin of this result, we measured the resistance between the arbitrary point on the channel and the source electrode by PCI-AFM. The low resistance region and high resistance region were clearly distinguished. These results suggest that the CNT network is divided into several islands which are connected with narrow conductive area. The results of the SGM are consistent with above results. [1] Q. Cao et al, Nature, 454 495 (2008). [2] T. Umesaka et al, Jpn. J. Appl. Phys., 46, 2496 (2007). [3] Y. Otsuka et al, Appl. Phys. Lett., 82 1944 (2003). [4] Y. Okigawa et al, Jpn. J. Appl. Phys., 49 02BD02 (2010). [5] T. Mizutani et al, NT08, D42.

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### Fabrication of freely suspended carbon nanotube and graphene devices

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Carbon nanotubes (CNTs) and graphene samples that are suspended have minimal interactions with the substrate and give therefore better possibilities to explore their intrinsic properties [1]. We realize our samples on thin Si3N4 membranes with a µm wide slit opening. Across the slit we deposit CNTs or graphene by first transforming it into a polyelectrolyte salt [2, 3], which is spontaneously dissolving in polar organic solvents without any sonication, use of surfactants or covalent functionalization that may be harmful to the carbon lattice. Deposition is then made either by spinning or with the help of dielectrophoresis [4]. The resulting samples make it possible to combine electrical transport measurements, optical spectroscopy and electron microscopy (TEM, electron diffraction) on the same individual CNT or graphene ribbon. The suspended nanotubes or graphene can be used for varied advanced applications, e.g. resonators or nano-sensors. [1] J. Cao, Q. Wang, H. Dai, Nature Mat. 4 (2005) 745. [2] A. Penicaud, et al., J. Am. Chem. Soc. 127 (2005) 8. [3] C. Vallés, et al., J. Am. Chem. Soc. 130 (2008) 15802. [4] A. Vijayaraghavan, et al., Nano Lett. 7 (2007) 1556.

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### Mechanical and electrical properties of SWCNT buckypaper and its composites

**Jingwen Guan**, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Canada* | **Yadienka Martinez-Rubi**, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Canada* | **Behnam Ashrafi**, *Institute for Aerospace Research, National Research Council Canada, Canada* | **Girjesh Dubey**, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Canada* | **Benoit Simard**, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Canada*

Single-walled carbon nanotubes (SWCNT) have very large aspect ratio and hence, like any fibrous materials, they can be assembled in paper like sheets, known as buckypaper (BP). BP has high potential in a wide range of applications including electrodes, gas separators, field emitters, actuators, sensors, electromagnetic shielding elements and reinforcing elements in composite structures. Buckypaper is commonly manufactured through filtration of a suspension of well dispersed SWCNT [1, 2]. SWCNT can be modified either before or after the buckypaper formation. In addition, the buckypaper can be impregnated with epoxy resins, polymers and bi- or trifunctional bridging agents to form 2D or 3D networks in situ. In this presentation, we will report the general techniques to manufacture BP with different lateral dimensions and thicknesses. BP has also been impregnated with epoxy resin, coated with polymers, and bridged with multi-functional bridging agents. Their mechanical properties and electrical conductivities have been thoroughly investigated and will be presented and discussed. [1] C.M. Aguirre, S. Auvray, S. Pigeon, R. Izquierdo, P. Desjardins, R. Martel, Appl. Phys. Lett. 2004, 88, 183104. [2] M.B. Jakubinek, M.B. Johnson, M.A. White, J. Guan, B. Simard, J. Nanosci. Nanotechnol. In press (2010).

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### Coupled thermogravimetry, mass spectrometry, and infrared spectroscopy for quantification of surface functionality on single-walled carbon nanotubes

**Christopher Kingston**, *National Research Council Canada, Steacie Institute for Molecular Sciences* | **Yadienka Martinez-Rubi**, *National Research Council Canada, Steacie Institute for Molecular Sciences* | **Jingwen Guan**, *National Research Council Canada, Steacie Institute for Molecular Sciences* | **Michael Barnes**, *National Research Council Canada, Steacie Institute for Molecular Sciences* | **Christine Brophy**, *National Research Council Canada, Institute for National Measurement Standards* | **Ralph Sturgeon**, *National Research Council Canada, Institute for National Measurement Standards* | **Benoit Simard**, *National Research Council Canada, Steacie Institute for Molecular Sciences*

We have successfully applied coupled thermogravimetry, mass spectrometry, and infrared spectroscopy to the quantification of surface functional groups on single-walled carbon nanotubes. A high-purity single-walled carbon nanotube sample was subjected to a rapid functionalization reaction that attached butyric acid moieties to the nanotube sidewalls. This sample was then subjected to thermal analysis under inert desorption conditions. Resultant infrared and mass spectrometric data were easily utilized to identify the desorption of the butyric acid groups across a narrow temperature range and we were able to calculate the degree of substitution of the attached acid groups within the nanotube backbone as 1.7 carbon atoms per hundred, in very good agreement with independent analytical measurements made by inductively coupled plasma optical emission spectrometry (ICP-OES). The thermal analysis technique was also able to discern the presence of secondary functional moieties on the nanotube samples that were not accessible by ICP-OES. This work demonstrates the potential of this technique for assessing the presence of multiple and diverse functional addends on the nanotube sidewalls, beyond just the principal groups targeted by the specific functionalization reaction.

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### Strain effect on polarized micro-Raman spectrum of vertically grown single-walled carbon nanotube forests

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Vertically grown single walled carbon nanotube (V-SWCNT) forests, synthesized by water assisted plasma enhanced chemical vapor deposition, were studied using polarized micro-Raman spectroscopy. Degree of V-SWCNT alignment along the vertical growth direction was investigated at three different sections (root, center, and end). Observed degree of V-SWCNT alignment was highest at the center part. G-band Raman frequency red-shift up to 13cm-1 and simultaneous line-width broadening were observed at the center part, as compared to those at the root and the end parts. Furthermore, G-band Raman frequency shift up to 8cm-1 was also observed when the same spot at the center part was measured with different polarization configurations, which can be attributed to strain effect. The observed strain effect was more pronounced for thicker regions at the center part of the V-SWNCT forests. (This work was supported by Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2009-0093817))

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### Photoluminescence on single-walled carbon nanotubes: A recipe to relative signal intensities

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Photoluminescence excitation (PLE) is a reliable and well established spectroscopic characterization tool in carbon nanotube (CNT) research. It reveals the presence, species and optical transition energies of semiconducting single-walled-CNTs in the lower diameter regime ~1nm. To study the chirality specific solubilisation efficiency of surfactants/molecules or to estimate the relative abundance of different species in a given sample, a reliable determination of the relative signal intensities is necessary. We propose a volume generated by the FWHM of PL, PLE and their mutual peak height as the appropriate measure, which leads to an intensity shift towards CNT species of lower diameters and higher chiral angles. Besides chirality specific PL properties, this is supported by a technical analysis focussing on PL spectrometers which use an incoherent light source for excitation: the FWHM of PLE is broadened depending on the optical transition energy of corresponding CNT species. The broadening may reach up to 11meV. In addition, we deliver a straight forward recipe to obtain the relative signal intensities as proposed above.

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### Phase transformation diagrams of iron nanowires confined in multi-walled carbon nanotubes

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Phase diagrams of materials at the nanoscale as for confined nanomaterials, are different from those of bulk materials: changes of transition temperatures and/or new phases could be expected. Their studies have a fundamental interest but may also have an interest for applications. We study here iron-based nanoparticles and nanowires confined inside carbon nanotubes (CNT). During CNT synthesis at 850°C by aerosol-assisted CCVD, CNT filling with nanoparticles and nanowires is occurring. Different iron-based phases are identified by X-ray diffraction (XRD) performed at room temperature: metallic alpha and gamma iron, oxide and carbide. This work is focused on the study of their phase diagram is studied by XRD in an oven, under vacuum, using synchrotron radiation (beamline DIFFABS, SOLEIL, France). Temperature cycling allowed us to evidence: reduction of iron oxide into alpha iron; partial transformation on cooling of gamma into alpha iron at a temperature much lower than that in the bulk, which could be an effect of the nanoscale. The occurrence however of residual gamma iron after thermal treatment is attributed to confinement effect since the gamma to alpha transformation implies a dilatation in two directions. We have also highlighted the liquefaction of iron nanowires at temperatures lower than those of macroscopic materials. These results, together with the comparison of thermal dilatation coefficients and Debye-Waller factors between bulk and nanomaterials, will be presented and discussed. Moreover this study underlines that thermal treatment allowed the formation of additional alpha iron, which is of strong interest for high density magnetic storage applications.

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### Imaging and Raman Spectroscopy Study of Individual Carbon Nanotubes Grown on Different Substrates

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Carbon nanotubes (CNTs) were synthesized in a vertical laminar flow reactor using supported catalyst particles in chemical vapor deposition processes aiming the controlled synthesis of single- and double-walled carbon nanotubes (SWCNTs and DWCNTs, respectively). Controlling the synthesis parameters was possible to promote the preferential growth of DWCNTs or SWCNTs. Appropriate synthesis conditions also led to the control of CNTs growth density producing isolated CNTs on the substrates rather than agglomerated nanotubes. Confocal Raman spectroscopy was used to characterize CNTs grown over different substrates. The main Raman active features of SWCNTs and DWCNTs are the radial breathing mode at low frequencies as well as G- and G'-band at high frequencies around 1590 and 2700 cm-1, respectively. Raman images were acquired in the range of 1560-1620 cm-1 probing the G-band of CNTs. The occurrence of failures on the images, similar to interruptions of the resonant signal along the nanotubes, was observed. Further acquisition of Raman images at lower frequencies ranges (1530-1560 cm-1) showed the absence of CNTs ruptures. Based on images, spectra were taken along the nanotubes. The Raman spectra profiles measured along the nanotubes indicated the occurrence of CNTs presenting structural distortions over the substrates. Raman characterization also showed the influence of the substrate on the growth of CNTs. The catalyst particle-substrate interaction can affect the growth process resulting in the formation of CNTs presenting different characteristics. Herein, was observed that sapphire substrate promoted the growth of CNTs with a high level of defects compared to the nanotubes obtained on quartz.

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### Thermal Conductivity of Single-Walled Carbon Nanotubes under Axial Stress

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Why do we study the thermal conductivity of carbon nanotubes (CNTs) under stress? First, the stress induced deformation has shown to change the electronic properties of CNTs. Thus it's necessary to study its thermal conductivity because the application in the nanoelectronics. Second, the phonon spectra changes when stress exerted on the CNTs, which helps us understanding the contribution of different kinds of phonon modes to the heat conduction. Thermal conductivity of the CNTs has a strong dependence on its length. However, how the length and boundary limit the phonon modes and the contribution of variety of phonon modes is not well understood. In this work, the thermal conductivity of SWCNTs under axial stress is studied by nonequilibrium molecular dynamics method. The thermal conductivity is found to increase and then decrease with the tube elongation changing from an axially compressed state to a stretched state. The phonon density of states of the systems is analyzed to elucidate the variation of heat conduction with respect to the stress in CNTs. The primary peak of the phonon spectrum shows a blue shift or red shift as the SWCNT is compressed or stretched. These shifts correspond to the change of the elasticity coefficient of the CNTs. The variation trend of primary peak height of radial phonon spectra with axial strain is similar to that of the thermal conductivity, which indicates that the radial phonon modes, especially the high-frequency modes, play a dominant role in the heat conduction mechanism of CNTs.

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### High Performance Resonance Raman Spectroscopy Using Volume Bragg Gratings as Tunable Light Filters

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We designed a NIR tunable resonance Raman spectroscopy system using a tandem of thick volume Bragg gratings (VBGs). VBGs are here the basic constituents of two light filtering units: a tunable laser line filter (LLF) and a tunable notch filter (NF). When included in a micro-Raman setup equipped with single stage monochromator with a 1800 gr/mm grating, the tandem of LLF and NF allowed measurements down to 20 cm-1. The fast tunability of the system was demonstrated on a bulk single-walled carbon nanotube sample through a series of 22 Stokes and anti-Stokes spectra recorded at excitation wavelengths between 800 nm and 990 nm. The main drawback of the setup is the limited angular acceptance of the filters (around 1 mrad), which causes mainly attenuation problems with the NF. The impact of this limitation is discussed.

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### Super growth of carbon nanotubes using water assisted chemical vapor deposition

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In this oral session, I will discuss the studies carried out at our group on the carbon nanotube growth using water assisted chemical vapor deposition (WA–CVD). The talk will include a) optimization of WA-CVD for the super growth of CNTs, b) alignment and wall control in CNTs, c) growth interruption studies, d) barrier layer mediated catalytic deactivation e) use of H2 for the infinite growth of CNTs, f) e-beam sensitive catalyst for patterned CNT growth g) from low pressure WA-CVD to atmospheric WA-CVD and h) some current studies like continuous CNT and yarn production.

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### Large Scale Production of vertically aligned CNT Films

**Ken Bosnick**, *NRC - NINT* | **Lei Dai**, *NRC - NINT*

Vertically aligned carbon nanotube (VACNT) films are among the morphologies of carbon nanotubes with the most promise for technological exploitation, but have previously only been produced in small quantities. We have successfully synthesized VACNT films on a multi-wafer scale in a commercial large-bore CVD reactor. The reactor is capable of processing batches as large as fifty 150 mm wafers simultaneously with all steps between loading and unloading fully automated. The films consist of densely packed and vertically aligned multiwalled carbon nanotubes. Metrology standards have been developed to facilitate process optimization and industrial quality control [1]. The growth kinetics in the large volume process were studied using the developed metrology and a Cr-Ni-Fe film stack as the catalyst. It is found that pre-growth treatment times of about 210 minutes are needed to reach steady state catalyst conditions. Shorter pre-growth treatment times produce a thicker but less dense film, without affecting the CNT diameter distribution. A catalyst activation model is proposed to explain these results. The general growth kinetics were studied under the steady state catalyst conditions [2]. [1] Lei Dai, Peter Wang, and Ken Bosnick, J. Vac. Sci. Technol. A 27(4), 1071 (2009). [2] Ken Bosnick and Lei Dai, J. Phys. Chem. C Articles ASAP (2009)

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### First-principles based kinetic modeling of effect of hydrogen on growth of carbon nanotubes

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The influence of hydrogen on the separate stages of carbon nanotube growth is investigated for thermal chemical vapor deposition. According to our kinetic calculations, during the delivery of carbon precursors by the gas flow, the precursors can be hydrogenated, thus leading to modification of the carbon supply rate onto the catalyst particle. A simple kinetic model of growth of CNTs based on the first-principles calculations of kinetic parameters for dissociation of hydrocarbons on the catalyst surface is suggested to study the hydrogen-modified adsorption/desorption kinetics of precursors on the Ni (111) and Ni (113) surfaces. Using the proposed model, conditions at which the growth of CNTs is possible are analyzed. Hydrogen is shown to decrease the coverage of hydrocarbons and thus prevent deactivation of the catalyst. Density functional theory calculations reveal that hydrogen adatoms effectively bind to edges of graphitic structures on the Ni (111) surface. This leads to a significant decrease of the rate of carbon attachment to the growing graphitic structures. The results obtained are shown to be in good agreement with the experimental data.

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### Mechanistic investigations of single-walled carbon nanotube synthesis by ferrocene vapor decomposition in carbon monoxide

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The single-walled carbon nanotubes (SWCNTs) were synthesized by the carbon monoxide disproportionation reaction on Fe catalyst particles formed by ferrocene vapor decomposition in a laminar flow aerosol (floating catalyst) reactor. On the basis of in situ sampling of the product collected at different locations in the reactor, kinetics of the SWCNT growth and catalyst particle crystallinity were studied. Catalyst particles captured before SWCNT nucleation as well as inactive particles were determined to have cementite (Fe3C) phase, while particles with fcc and bcc Fe phases were found to be embedded in the SCWNTs. The growth rate in the temperature range from 804 to 915 °C was respectively varied from 0.67 to 2.7 μm/s. The growth rate constant can be described by an Arrhenius dependence with an activation energy of Ea = 1.39 eV, which was attributed to the carbon diffusion in solid iron particles. CNT growth termination was explained by solid-liquid phase transition in the catalyst particles. A high temperature gradient in the reactor was found to not have any effect on the diameter during the SWCNT growth and as a result on the chirality of the growing SWCNTs. The mechanism of SWCNT nucleation and growth was proposed.

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### CCVD synthesis of carbon-encapsulated metal nanoparticles for hyperthermia

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This work was performed in the frame of the European FP6 RTN CARBIO (www.carbio.eu, bio-application of carbon nanotubes filled with magnetic materials for cancer treatment by hyperthermia). Earlier work demonstrated that it is possible to tightly encapsulate Co nanoparticules in carbon shells [1]. Here, we report the synthesis of carbon-encapsulated metal (Fe, Co) nanoparticles (CEMNP) by catalytic chemical vapour deposition (CCVD) and the results of magnetic and hyperthermia measurements. The CEMNP have been synthesized by catalytic chemical vapour deposition (CCVD) with mixtures of H2/CH4 or N2/CH4, using Mg0.95Co0.05O [2] or Mg0.95Fe0.05O solid solutions as catalysts. Some particles are encapsulated in graphitic shells while others are located inside hollow carbon nanofibres. The samples contain either spherical and oblong carbon-encapsulated Co nanoparticles with diameter within the range 10 - 15 nm or oblong or spherical carbon-encapsulated Fe nanoparticles with diameter within the range 10-20 nm, depending on CCVD conditions. Metal content in the final purified products were 10 – 11 wt.% of Co or 7 – 13 wt.% of Fe. The magnetic characterization of carbon-encapsulated Co nanoparticles shows high magnetization and heating effect (suspension in water) was evidenced at 30 kA/m and rather low concentration (5mg/mL). Recent measurements also show that there is significant heating at 119 kHz. The samples were also characterized by TEM, Raman spectroscopy, elemental analyses, X-ray diffraction, SQUID magnetometer, AGM and AC- magnetic field. References: [1] E. Flahaut, et al., Chem. Mater., 14, (2002), 2553 [2] E. Flahaut et al., J. Mater. Chem., 10, (2000), 249

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### Patterning of carbon nanotube structures through a chemical imprint strategy

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The patterning of carbon nanotube (CNT) arrays was of common interest due to the promising applications. Conventionally, the patterning of CNT growth involved the patterning of catalyst films, which needs relatively complex procedures such as lithography or ultraviolet exposure. Herein, we reported that the patterning of CNT arrays can be simply realized through the chemical masks with different compositions. Planar micro-patterned grids were used as masks and were laid onto the substrates to assist the patterned growth of CNTs. Covering of the masks realized the patterning of CNT arrays by facilitating or limiting the CNT growth under the covered area. XPS analysis confirmed the migration of chemical components from masks onto substrates, which was responsible for the patterning effect. When the promoters (like Mo grids) were laid on substrate, patterned Mo components were imprinted onto substrate through sublimation. Mo and original Fe catalyst showed synergetic effect, which enhanced the growth of CNT arrays. Therefore, the rilievi-structured CNT array pattern can be obtained. By varying the thickness of Fe catalyst layer and the annealing conditions, the structure of CNT array patterns can be readily modulated. Contrarily, the inhibitor masks may deactivate the Fe catalyst layers and lead to the formation of intaglio-structured CNT array patterns. As the chemical masks of various materials can be facilely obtained through the micro-machining, this method brings a feasible route to control the nanoscale self-assembling of CNT structures. Based on this process, super-hydrophobic patterned CNT structures with a contact angle of 152o can be fabricated.

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### Horizontally Aligned SWNT Growth on R-cut Crystal Quartz Substrates

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Orientation control of SWNTs is important for the fabrication of SWNT applications. Horizontally aligned SWNTs can be synthesized on specific substrates, such as sapphire and crystal quartz substrates, and ST-cut substrates are popularly used in the case of crystal quartz substrates. On ST-cut surfaces, SWNTs are grown along the direction of the x-axis, and the orientation is improved after the substrates are annealed at high temperature for an extended time. The orientation mechanism is understood by the atomic structure of the ST-cut surface. However, the ST-cut surface is complicated because it is an artificial surface. In this paper, we used R-cut ([101] face) substrates of crystal quartz for horizontal aligned growth of SWNTs. The [101] face is one of the stable surfaces that appear on natural quartz crystal, and it is closest to the structure of the ST-cut surface. Fe/Co metal nanoparticles supported on zeolite particles were used as catalyst. The zeolite particles were dispersed on the R-cut surface and SWNTs were synthesized by the alcohol catalytic CVD method. SEM and AFM observations revealed that SWNTs were grown along the direction of the x-axis on the R-cut surface without annealing treatment. On the R-cut surface, step and terrace structures appeared in AFM images. SWNTs were aligned in the terraced area, indicating that this surface structure aligned the SWNTs. We conclude that the ST-cut surface is a collective of small domains of [101] faces and the resulting alignment of SWNTs is owing to the [101] face structure.

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### Growth of high-density vertically-aligned carbon nanotubes on conductive substrates by plasma-assisted catalyst pretreatments

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A plasma-assisted thermal pretreatment of Ni, Co, or Fe films facilitates the growth of high-density vertically-aligned arrays of small diameter carbon nanotubes on conductive materials such as TiN or doped mono- and poly-crystalline Si. The plasma-assisted pretreatment promotes stronger catalyst-support interactions than the purely-thermal pretreatment. This reduces catalyst mobility and hence stabilizes smaller catalyst particles with a higher number density. Purely-thermal catalyst pretreatment gives limited or no growth on these substrates.

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### Synthesis of B-doped DWCNTs using catalytic reaction of triisopropyl borate

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Although CNTs have outstanding properties for applications such as electronic devices, field emitter, transparent conducting film, sensor, one of the greatest challenges, the tailoring of their electronic properties remains unfulfilled. In particular, the separation of metallic and semiconducting CNTs is still needed. One candidate method to tailor the electronic properties is to chemically modify the CNTs by substitution of the carbon atoms with the incorporation of heteroatom like boron into the carbon networks. B-doped CNTs all reveals a metallic behavior irrespective of diameter or chirality, because the substitution of boron atom in hexagonal carbon lattice gives rise to acceptor states near the Fermi level of the material. In this communication, we demonstrate the synthesis of high-quality B-doped DWCNTs by catalytic decomposition of tetrahydrofuran and triisopropyl borate over Fe-Mo/MgO catalyst at 900 ¡É. An overall observation in our products indicates that proportion of synthesized DWCNTs was approximately over 90 % and SWCNTs very few exist below 10 % in the as-grown carbon products. From XPS result, the B-C bonding in B1s signals provide evidence for highly coordinated boron atoms replacing carbon atoms within the graphite sheet. We obtained substituted boron concentration of 0.9 - 2.8 at.% according to increasing triisopropyl borate concentration of 20 - 60 %. We suggest that substituted boron concentration in the hexagonal carbon lattices can be easily controlled by concentration of triisopropyl borate. We designed flexible transparent conducting film using B-doped DWCNTs.

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### Study of relationship between diameter of carbon nanotubes and surface morphology of Al2O3 supporting layer

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It is widely recognized that single-walled carbon nanotubes (SWNTs) has emerged as alternative material for next-generation electronics owing to extraordinary electrical properties associated with one-dimensional nature. Since the electronic properties of SWNTs depend on their geometrical structures such as chirality and diameter, controlling SWNTs diameter is thus considered as an ultimate goal for application of SWNTs-based nanoelectronics. It is well known that the SWNTs diameter can be influenced by a catalytic nanoparticle size. Here, we systemically investigated the relationship between the SWNTs diameter and surface morphology of Al2O3 supporting layer. The SWNTs were synthesized on a nanostructured catalytic layer consisting of Fe/Al2O3/Si substrate using a conventional thermal chemical vapor deposition system. The morphological and chemical features of Al2O3 layer and Fe catalytic nanoparticles were studied by atomic force microscopy, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy. The characterization of SWNTs was conducted by SEM and resonant Raman spectroscopy with excitation wavelengths of 514 nm (2.41 eV) and 633 nm (1.96 eV). As a result, the RMS roughness and grain size of Al2O3 layer can be controlled by adjusting thickness of Al layer. The agglomeration induced by surface diffusion of Fe catalytic nanoparticles can be governed by the structural modification of Al2O3 layer, which gives rise to change in SWNTs diameter. In the case of 15-nm-thick Al2O3 layer, the synthesis of SWNTs with an extremely narrow diameter distribution was achieved successfully.

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### Synthesis, characterization and physical properties of Co@Au core-shell nanoparticles encapsulated in N-doped multiwall carbon nanotubes

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Au/Co thin films were deposited on silicon substrates using the magnetron sputtering method. The Au/Co nanostructured films were then used as catalytic support to grow nitrogen-doped carbon nanotubes (CNx) via chemical vapor deposition (CVD) at 850 °C, involving benzylamine (C6H5CH2NH2) as a carbon and nitrogen sources. The resulting material was identified as CNx nanotubes containing Co@Au core-shell nanoparticles inside their tips. We performed a careful characterization using scanning and transmission electron microscopy (SEM & TEM), X-ray diffraction, thermogravimetric analysis (TGA), magnetic measurements, and electric transport. We noted that the metal particle cores consist of cobalt (ca. 80-nm diameter) and the Au shell exhibited a thickness of ca. 5 nm. Magnetic measurements revealed a ferromagnetic behavior of the system composed of Co@Au nanoparticles encapsulated inside multi-walled carbon nanotubes (MWNTs), and a negative magnetoresistence at low temperatures. The results are compared with pristine CNx MWNTs containing pure Fe nanoparticles encapsulated in their cores.

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### Catalyzed growth of carbon nanotubes by hybrid molecular dynamics / force biased Monte Carlo simulations

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To gain insight into the metal catalyzed growth mechanisms of single-walled carbon nanotubes (SWNT), SWNT cap formation was studied by hybrid molecular dynamics / uniform acceptance force biased Monte Carlo (md/UFMC) simulations using the recently developed ReaxFF reactive force field. Using this novel approach, allowing the incorporation of relaxation effects, a step-by-step atomistic description of the nucleation process is presented. It is shown how the formation of two caps proceeds by a root growth mechanism and a third cap developes by a tip growth mechanism. Furthermore, the importance of the relaxation of the network is highlighted by these results.

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### Catalyst and Chirality Dependent Growth of Single-Wall Carbon Nanotubes Determined Through Nano Test Tube Chemistry

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and molecules. Using this unique nano environment for a test tube experiment allows chemical reactions to be confined at the nanoscale where novel chemistry processes can occur and individual chemistry events can be observed at the molecular level [1,2]. The inside of carbon nanotubes is clean and encapsulated precursor compounds provide elemental sources in a designer proportion. In this contribution the excitement of nano test tube chemistry is exemplified on the growth of inner tubes from encapsulated molecules. Using various filling precursors we study the mechanism for the growth of carbon nanotubes. In our recent work two model catalysts, Fe and Pt, were prepared together with carbon feedstock via filling of original single wall tubes with ferrocene and Pt(II) acetylacetonate, respectively. These filled single-wall tubes were then converted into double-wall carbon nanotubes via thermal annealing in vacuum. A combination of Raman spectroscopy and transmission electron microscopy allowed precise and quantitative information of the growth properties to be obtained. Details of determined activation temperatures for specific chirality tubes and catalysts will be presented. Such information would be fundamental to possibly exercise control of chirality on the growth of carbon nanotubes on the bulk scale. [1]. H. Shiozawa et al., Adv. Mater. 20, 1443 (2008). [2]. H. Shiozawa et al., Phys. Rev. Lett. 102, 046804 (2009).

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### Searching for carbon nanotubes of one type through solid state diacetylene polymerization

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All known procedures to synthesize carbon nanotubes yield a mixture of nanotubes with different chiralities and diameters, thereby resulting in materials with uncontrolled electronic and optical properties that limit their applications. Efforts to control the diameter through zeolite templating1 still yield mixtures of few chiralities. We have previously proposed a topochemical route for the rational synthesis of single wall carbon nanotubes of one type by employing the solid state polymerization of cyclic diacetylenes2. One of the challenges related to this approach is the obtention of crystals with the appropriate stacking arrangement for 1,4-addition polymerization that yield these organic nanotubes. In this work, we present and discuss the results of our research regarding the preparation and characterization of these organic nanotubes. References: .N. Wang, Z. K. Tang, G. D. Li, J. S. Chen, Nature (2000) 408 50. 2. R. H. Baughman, M.C. Biewer, J.P. Ferraris, J.S. Lamba, Synth. Metals (2004) 141 87.

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### Efficient Anchoring of Nanostructured Cadmium Selenide on Nitrogen Doped Carbon Nanotubes

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We report efficient coating of nitrogen doped carbon nanotubes (CNx-MWNTs) with Cadmium Selenide (CdSe) after optimizing reaction conditions for the in-situ synthesis of this semiconductor. We tested different reaction media (methanol, isopropanol, water) and the use of sonication to optimize dispersion, as well as the effects of temperature, and reactants in the synthesis. Electron microscopy (SEM, STEM, TEM) was used to verify the dispersion and uniformity of the CdSe coating over the nanotubes. We have found that since CNx are by nature more reactive they need not be functionalized for CdSe to deposit over them as it is synthesized, yielding tubes coated with nanoparticles and sheaths of CdSe. When CdSe nanoparticles are just mixed with CNx they are not anchored efficiently. We have obtained very good results in aqueous solutions making this more environmentally friendly than organic solvent based processes. The CdSe-CNx composite material can have application in photovoltaic devices, since CNx are good electrical conductors.

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### Influence of graphitic structure of anode on synthesis of single-walled carbon nanotubes using a direct current arc discharge method

**Hikaru Nishizaka**, *Tohoku University* | **Yoshinori Sato**, *Tohoku University; PRESTO, Japan Science and Technology Agency* | **Kenichi Motomiya**, *Tohoku University* | **Kazuyuki Tohji**, *Tohoku University*

The soot synthesized by a direct current arc discharge method contains SWCNTs and a variety of impurities including graphite, metal nanoparticles, graphite coated metal clusters, amorphous carbon, and other carbon compounds such as fullerenes. In our laboratory, the easy and high yield purification method of SWCNTs have been developed combining air oxidation and acid treatment. However, the graphite remains in the purified SWCNTs, which comes from the graphite anode. Here, we report on the influence of graphitic structure of anode on synthesis of SWCNTs using a direct current arc discharge by changing a carbon material of anode. In this study, two anodes were used, which possess each different graphitic structure, that is, graphite and carbon black (CB) rod, respectively. SWCNTs with very few graphite impurities were obtained using CB rod. The yield and structure of the synthesized carbonous impurities were found to be strongly influenced by the fine and graphitic structure of anode. The graphitic structure of anode affected not only the yield but also the selective of synthesis with a given diameter of SWCNTs. Content of graphitic impurities in the synthesized SWCNT soot increased with increasing arc current density. One of the reasons on the contamination of graphitic impurities into the synthesized SWCNT soot is confirmed to be caused by sputtering anode. We demonstrated that this method, arc discharge method using an amorphous carbon anode, was an effective solution to synthesize SWCNTs with few graphite impurities.

## Thursday, July 1

### 15:33-17:00 Poster Session 5

### Poster Board | 5

**Characterization of Thin Film Transistor Using As-grown Single-walled Carbon Nanotubes from Dip-coated Catalyst by Patterned Removal of Self-assembled Monolayer**

**Shinya Aikawa**, *University of Tokyo; Tokyo University of Science* | **Rong Xiang**, *University of Tokyo* | **Erik Einarsson**, *University of Tokyo* | **Asahi Kitabatake**, *University of Tokyo* | **Shohei Chiashi**, *University of Tokyo* | **Junichiro Shiomi**, *University of Tokyo* | **Eiichi Nishikawa**, *Tokyo University of Science* | **Shigeo Maruyama**, *University of Tokyo*

A carbon nanotube field effect transistor (CNT-FET) having a single-walled carbon nanotube (SWNT) as its gate channel has been investigated because of its potential applications in next-generation nanoscale organic electronic devices. However, the fabrication process using conventional MEMS techniques has many steps and it limits catalyst coating method to a dry process, such as vacuum evaporation. We previously reported that it is possible to pattern the growth of SWNTs using a wet process such as dip-coating by making hydrophilic and hydrophobic regions on a substrate surface [1]. In this study, we fabricated and evaluated the performance of a thin film transistor consisting only of as-grown SWNTs by selectively removing a self-assembled monolayer (SAM) from the catalyst deposition area. An octadecyltrichlorosilane SAM was used to make pattern on a Si substrate as follows: The SAM was formed on an OH-terminated Si surface and was selectively removed by vacuum ultraviolet (VUV) irradiation through a photomask to pattern the substrate. After SAM removal, the substrate was dipped into a Co solution to deposit catalyst [2], and SWNTs were grown by alcohol CVD (ACCVD) [3] only in the regions that had been irradiated by VUV. The I-V characteristics were measured using the Si substrate as a back-gate and the SWNT pads as source/drain electrode. The I-V characteristics of the fabricated device and possibility of transfer to a flexible substrate will be discussed. [1] JACS. 131, 10344 (2009). [2] CPL. Lett. 377, 49 (2003). [3] CPL. 360, 229 (2002).

### Poster Board | 8

**Field alignment of carbon nanotubes during growth and emission**

**Grigory Bocharov**, *Kintech Lab Ltd, Moscow, Russia* | **Andrey Knizhnik**, *Kintech Lab Ltd, Moscow, Russia* | **Alexander Eletskiy**, *Kintech Lab Ltd, Moscow, Russia* | **Timothy Sommerer**, *GE Global Research, Niskayuna, USA*

The inter-relation between the orientation angle of a tilted carbon nanotube and applied electrical field strength has been derived. In accordance to this relation, the resulting orientation angle is determined on the basis of the mechanical balance between the electric torque and the elastic mechanical torque. This inter-relation is used for evaluation of the I-V characteristics of a CNT-based cathode consisted of initially tilted nanotubes. The degree of deviation of these characteristics from the conventional Fowler-Nordheim function depends on both the average initial tilting angle of nanotubes and the Young modulus of the nanotubes. Contact potential difference caused by a difference in the electron work functions between the nanotube and the substrate results in charging the nanotubes which causes the self-tilting of CNTs comprising the array. The angle of self-tilting increases as the distance of the center of the array increases. Taking into account self-tilting of CNTs due to the contact potential difference changes the current-voltage characteristic of an array so that the optimum inter-tube distance depends on the average electrical field strength.

### Poster Board | 11

**Stability of Transparent SWNTs and DWNTs Network Films**

**Seung Bo Yang**, *KAIST*

We studied the stability of single-walled carbon nanotube (SWNT) and double-walled carbon nanotube (DWNT) films as a function of surface modification. Conductivity measurements disclosed that gold ion and HNO3 treatment of the nanotube network films increased the electrical conductivity by more than a factor of 2 with negligible loss of transmittance. However, the long-term stability of the films varied depending on nanotube type and post-treatment method, with gold ion-treated nanotubes exhibiting higher stability than HNO3-treated nanotubes. Moreover, DWNTs showed better stability than SWNTs when treated with gold ions. Work function and optical absorption spectral measurements suggested that the dedoping process and the contact resistance of the nanotube networks may be important for stability under ambient conditions. These results are important for the development of surface-modified SWNTs and DWNTs for potential applications in solar cells, light-emitting diodes, sensors, and field-effect transistors.

### Poster Board | 17

**Unbundled semiconducting single-wall carbon nanotubes for thin film transistors**

**Yasumitsu Miyata**, *Department of Chemistry, Nagoya University, Japan* | **Kazunari Shiozawa**, *Department of Chemistry, Nagoya University, Japan* | **Yuki Asada**, *Department of Chemistry, Nagoya University, Japan* | **Ryo Kitaura**, *Department of Chemistry, Nagoya University, Japan* | **Yutaka Ohno**, *Department of Quantum Engineering, Nagoya University, Japan* | **Takashi Mizutani**, *Department of Quantum Engineering, Nagoya University, Japan* | **Hisanori Shinohara**, *Department of Chemistry, Nagoya University, Japan*

Single-wall carbon nanotubes (SWCNTs) are expected as a promising material for thin film transistors (TFTs) because of their high carrier mobility, flexibility, and solution processability. Recently, we have reported a fabrication method of the networks of purely unbundled SWCNTs, and these networks show a high transistor performance even without the removal of metallic SWCNTs [1]. For further improvements, the use of highly-pure semiconducting SWCNTs is desirable. In this study, we have fabricated the TFTs using the networks of unbundled semiconducting SWCNTs. The SWCNTs were purchased from Meijo Inc. (So-type) and used as a starting material. Semiconducting SWCNTs were separated by using gel chromatography [2,3]. To fabricate TFTs, the sample solution was displayed on an amino-coated Si/SiO2 substrate, followed by the deposition of Ti/Au electrodes. The device has an on/off ratio of ~10^6 and a mobility of ~3 cm2V-1s-1. In this presentation, a detailed comparison of TFT characteristics between the pristine and the separated samples will be discussed. [1] Y. Asada et al. Adv. Mater. in press. [2] K. Moshammer et al., Nano Res., 2, 599 (2009) [3] T. Tanaka et al., Appl. Phys. Express, 2, 125002 (2009)

### Poster Board | 20

**New characteristics of carbon nanotube networks in electrolytes**

**Thurid Gspann**, *Institute for Applied Computer Science, KIT - Karlsruhe Institute of Technology, Germany* | **Ulrich Gengenbach**, *Institute for Applied Computer Science, KIT - Karlsruhe Institute of Technology, Germany* | **Michael Hanko**, *Endress + Hauser Conducta GmbH + Co. KG, Gerlingen, Germany* | **Manfred Jagiella**, *Endress + Hauser Conducta GmbH + Co. KG, Gerlingen, Germany* | **Georg Bretthauer**, *Institute for Applied Computer Science, KIT - Karlsruhe Institute of Technology, Germany*

For applications in sensor devices carbon nanotube field effect transistors are of great interest due to the remarkable electronic characteristics of the nanotubes. Many of the published devices are single-tube transistors that are laborious to produce and very susceptible to defects of the one connected nanotube. We report on easily and reproducibly manufactured devices and their electronic behaviour when gated through an electrolyte by an immersed reference electrode. The devices are based on filtered nanotube networks, made from 95% semiconducting nanotube material [1] and additionally optimized by light-induced modification loosely based on [2]. So we conquered the risk of perturbing metallic channels between the electrodes as well as the dependence on the characteristics of one particular nanotube. These devices can be used either directly in contact with an electrolyte or coated with a thin insulating layer for special sensing applications. The current through the nanotube networks changes significantly depending on the surrounding electrolyte. References [1] M. Arnold, A. Green, J. Hulvat, S. Stupp, M. Hersam, Nature Nanotechnology 1, 60 - 65 (2006) [2] L. Gomez, A. Kumar, Y. Zhang, K. Ryu, A. Badmaev, C. Zhou, Nano Letters 9, 3592 - 3598 (2009)

## Poster Board | 23

### Polymer/carbon nanoparticle composite strain sensors

**Samuel T. Buschhorn**, *TU Hamburg-Harburg* | **Christian Viets**, *TU Hamburg-Harburg* | **Luis A. S. A. Prado**, *TU Hamburg-Harburg* | **Jan Sumfleth**, *TU Hamburg-Harburg* | **Karl Schulte**, *TU Hamburg-Harburg*

Due to the combination of several outstanding properties nanotube based sensors are now being intensively researched. Advances have been made on a broad front of applications, be it detecting or distinguishing of substances or sensing of strain. This work presents recent achievements in strain sensing, specifically using the piezoresistive properties of a carbon nanoparticle based composites for monitoring structural integrity. A composite's piezoresistive properties may be influenced by a number of parameters such as particle shape, size, concentration, dispersion and external influences such as moisture, temperature, and of course strain. Nanocomposites have already shown high potential regarding sensitivity and hold additional advantages over currently used sensors based on fiber optics and metal-foils. Especially for device integration and adjustability the aforementioned parameters can be used to tune the sensor characteristics and improve its operational range. In this work a series of piezoresistive measurements were carried out for small and large strains to assess the change for different particle types (CB, CNTs, Graphene) and combinations. Different concentrations were tested, and material preparation and conditioning was varied to elucidate its influence. WAXS and SAXS measurements were conducted to determine particle orientation change upon strain and distribution in the sample. The results show that not only particle type but also dispersion play an important role. Furthermore it could be shown that tunnelling contacts and geometrical arrangement become increasingly important at high strain. As the principal influences are understood in more detail they can be used to manipulate the sensors characteristics for technical applications.

## Poster Board | 26

### Low resistivity interconnexions using double-walled carbon nanotubes (DWNT)

**Florent Seichepine**, *Université de Toulouse ; UPS, INP ; Institut Carnot Cirimat ; France; Université de Toulouse ; UPS, INSA, INP, ISAE ; LAAS ; France* | **Christophe Vieu**, *Université de Toulouse ; UPS, INSA, INP, ISAE ; LAAS ; France* | **Emmanuel Flahaut**, *Université de Toulouse ; UPS, INP ; Institut Carnot Cirimat ; France; CNRS ; Institut Carnot Cirimat ; France*

Carbon nanotubes (CNT) can be used for different applications in nanoelectronics. CCVD Double-walled CNT (DWNT) [1] have been shown to contain a high ratio of metallic nanotubes [2] and are thus very promising for use as interconnexions. We have investigated the electrical characterisation of deposits of DWNT using in-house test structures (set of electrodes) obtained by classic photolithography. The main advantage of our setup is the possibility to obtain quickly the electrical parameters from I(V) curves of large assemblies of DWNT (individual or in bundles).We are then able to identify individual 'events' (resulting from the burning of individual conduction ways), and to estimate for example the maximum current density of the corresponding CNT or bundle of CNT. The influence of electrode geometry and length was also taken into consideration. Results obtained with DWNT show that maximum current densities around 1E9 A/cm$^2$ can be easily reached and confirm the potential of this category of CNT as interconnexions. Moreover, the method enables to get information quickly about the distribution of the electrical properties of individual nano-objects (individual CNT or bundles of CNBT) in a given sample, thus allowing the comparison of different samples of CNT at a more macroscopic scale. References: [1] E. Flahaut et al., Chem. Comm. (2003) 1442 [2] P. Puech et al., Phys. Rev. B, 78, (4), (2008), 045413:1-6

## Poster Board | 32

### Carbon nanotube films fabricated by a simple transfer method and their electrical properties

**Doo Hee Hwang**, *Department of Micro/Nano Systems, Korea University* | **Ki Nam Yun**, *School of Electrical Engineering, Korea University* | **Dong Kyu Jang**, *School of Electrical Engineering, Korea University* | **Sun Kug Kim**, *School of Electrical Engineering, Korea University* | **Siegmar Roth**, *School of Electrical Engineering, Korea University* | **Cheol Jin Lee**, *Department of Micro/Nano Systems, Korea University; School of Electrical Engineering, Korea University*

As CNT devices have been attracted for various applications especially on flexible electronics, various techniques to fabricate the single-walled carbon nanotube (SWCNT) films on flexible substrates have been developed. However, most of these techniques have some limits due to their homogeneity, repeatability and complexity. We developed a simple fabrication method for the SWCNT film on the plastic substrate using a transfer method. The SWCNT was dispersed in 1,2-dichlorobenzene. Using a vacuum filtration method with an alumina oxide membrane, the SWCNT film was fabricated on the surface of the membrane. The SWCNT film was slowly dipped into the nitric acid in order to separate the SWCNT film from the membrane. Then, the SWCNT film separated in the nitric acid was transferred on a target substrate. Finally the transferred SWCNT film was dried in air ambient. SEM observation showed excellent transfer of the SWCNT film without any significant damage. The electrical conductivity of the transferred SWCNT film was improved compared with the pristine SWCNT film. In detail, the sheet resistance of the SWCNT film was changed from a 150~300 Ohm/sq to a 80~150 Ohm/sq at the transmittance of 70~80% after transferring the SWCNT film. This result is attributed to densification of the SWCNT network during a transfer process. We suggest that the transfer method provides a simple, controllable, and cost effective way to open up new possibility for flexible electronics

## Poster Board | 35

### Electron Counting Spectroscopy Technique

**Mariusz Zdrojek**, *ICN, Campus UAB, Spain* | **Maria Jose Esplandiu**, *ICN, Campus UAB, Spain* | **Adrian Bachtold**, *ICN, Campus UAB, Spain*

A new technique, electron counting spectroscopy has been used to probe the electronic properties of semiconducting CdSe quantum dots [1]. This technique allows us to fill or empty a semiconducting quantum dot with many electrons. The ability to shift the Fermi energy by a large amount holds promise for nanoscale or molecular electronics, since the large energy separation between the levels often has limited access to only few levels. The detection scheme is based on an original approach where the investigated particle is attached to only one electrode, a carbon nanotube. The conductance of the nanotube is measured as a function of a gate voltage (Vg), which allows the detection of individual electrons transferred onto the quantum dot. The electron transfer occurs only when the electrochemical potential of the nanotube matches the energy levels in the particle, while sweeping the gate voltage. We noticed no electron transfer for certain range of Vg which is attributed to the energy gap of the CdSe quantum dot. Our study shows that single-electron detection with CNT transistor represents a new strategy to study the separation in energy between the electronic discrete levels of the semiconducting quantum dot. In particular, it allows the study of the chaotic behavior of the electronic levels in the CdSe particle [1]. Additionally, we discuss the possibility of applying electron counting spectroscopy to investigate other type of quantum dots, e.g. gold nanoparticles and ferritin molecules (iron core protein). [1] M. Zdrojek et al., Phys. Rev. Lett., 102, 228604 (2009)

## Poster Board | 38

### Carbon Nanotube programmable devices for adaptive architectures

**Guillaume Agnus**, *CEA, IRAMIS, Service de Physique de L'Etat Condensé (CNRS URA 2464), Laboratoire d'Electronique Moléculaire, France* | **David Brunel**, *CEA, IRAMIS, Service de Physique de L'Etat Condensé (CNRS URA 2464), Laboratoire d'Electronique Moléculaire, France* | **Weisheng Zhao**, *CEA, LIST (Laboratoire d' Intégration des Systèmes et des Technologies),France* | **Karim Gacem**, *CEA, IRAMIS, Service de Physique de L'Etat Condensé (CNRS URA 2464), Laboratoire d'Electronique Moléculaire, France* | **Arianna Filoramo**, *CEA, IRAMIS, Service de Physique de L'Etat Condensé (CNRS URA 2464), Laboratoire d'Electronique Moléculaire, France* | **Stéphane Lenfant**, *IEMN, CNRS, Molecular Nanostructures and Devices Group, France* | **Dominique Vuillaume**, *IEMN, CNRS, Molecular Nanostructures and Devices Group, France* | **Christian Gamrat**, *CEA, LIST (Laboratoire d' Intégration des Systèmes et des Technologies),France* | **Jean-Philippe Bourgoin**, *CEA, IRAMIS, Service de Physique de L'Etat Condensé (CNRS URA 2464), Laboratoire d'Electronique Moléculaire, France* | **Vincent Derycke**, *CEA, IRAMIS, Service de Physique de L'Etat Condensé (CNRS URA 2464), Laboratoire d'Electronique Moléculaire, France*

Nano-objects such as carbon nanotubes are of great interest for the development of new generation of circuits the functionality of which could advantageously complement CMOS. However, conventional circuit architectures are not suited for nano-devices as the can barely cope with defects and variability. Conversely, neural networks represent a challenging approach which could take advantage of the rich functionality of nano-objects and at the same time handle variability. In this context, we showed that optically-gated carbon nanotube field effect transistors (OG-CNTFETs) [1,2] have all the required characteristics of artificial synapses, the basic building block for adaptive circuits [3]. They can be operated as 2-terminal devices with memory capabilities, large dynamics, high programming speed and tolerance to variability. In this work, we notably present nanotube network-based OG-CNTFETs the resistivity of which can be adjusted within 3 orders of magnitude at constant gate bias and then maintained in a non volatile way. Programming in the sub-µs time range is made possible through aggressive scaling of the gate dielectric. A way to implement these synapses in circuits with parallel learning capabilities and CMOS compatibility is also proposed [4]. Recent work on the lateral down-scaling of such architecture toward the realization of single nanotube perceptrons will also be presented. [1] J. Borghetti et al, Adv. Mater., 18 (2006) 2535. [2] C. Anghel et al, Nano Letters, 8 (2008) 3619. [3] G. Agnus et al, Adv. Mater. 21 (2009) 21. [4] Zhao et al, Nanotechnology, in press (2010).

## Poster Board | 41

### Controlling electronic and transport properties of double-wall carbon nanotubes

**Rodrigo Amorim**, *Universidade Federal do ABC - UFABC* | **Antônio da Silva**, *Universidade de São Paulo - USP; Laboratório Nacional de Luz Sínclotron* | **Adalberto Fazzio**, *Universidade de São Paulo - USP* | **Alexandre Rocha**, *Universidade Federal do ABC - UFABC*

Carbon Nanotubes (CNTs) have several unique properties such as the possibility of being metal or semiconductor, depending on its chirality, as well a large Young's Modulus (about 1TPa). One could alter the properties of CNTs either by synthesis/growth processes - in particular using an arch-discharge methods - or via ion irradiation. Experimental studies have shown that low doses of ion irradiation can create links between the walls of multiwall nanotubes and consequently modify the proprieties of CNTs, in particular their mechanical properties. The objective of this work is to investigate the electronic and transport properties of double-wall carbon nanotubes with defects forming links between their walls. We address two types of defects, namely the Wigner Defect –consisting of the Franckel pair composed by a pair vacancy-interstice - and a vacancy-vacancy defect. We discuss the stability of these tubes with crosslinks and how these defects could alter the electronic structure of the CNTs in two distinct concentrations (rho=0.082 def. Å-1 and rho=0.164 def. Å-1). Finally, we will show transport simulations to demonstrate conductance signature in double wall CNTs when the walls are connected by the links and how the nature of the electrodes influence on these results.

## Poster Board | 44

### Single Coaxial Nanowire Photovoltaic Device with Carbon Nanotube Core and Amorphous Silicon Shell

**Hang Zhou**, *Electrical Engineering Division and Center for Advanced Photonic and Electronics, Engineering Department, University Of Cambridge* | **George Lentaris**, *Electrical Engineering Division and Center for Advanced Photonic and Electronics, Engineering Department, University Of Cambridge* | **Pritesh Hiralal**, *Electrical Engineering Division and Center for Advanced Photonic and Electronics, Engineering Department, University Of Cambridge* | **Tim Butler**, *Electrical Engineering Division and Center for Advanced Photonic and Electronics, Engineering Department, University Of Cambridge* | **Gehan Amaratunga**, *Electrical Engineering Division and Center for Advanced Photonic and Electronics, Engineering Department, University Of Cambridge* | **Alan Colli**, *Cambridge Nokia Research Center*

Carbon nanotube is one of the promising materials for exploring new concepts in solar energy conversion and photon detection. Here, we report the first experimental realization of a single coaxial nanowire photovoltaic device (2-4µm) based on carbon nanotube and amorphous silicon. Specifically, a multi-walled carbon nanotube was utilized as the metallic core, on which n-type and intrinsic amorphous silicon layers were coated. A Schottky junction was formed by sputtering a transparent conducting indium-tin-oxide layer to wrap the outer shell of the device. The single coaxial nanowire device showed typical diode ratifying properties with turn-on voltage around 1V and a rectification ratio of ~104 when biased at ±2V. Under illumination (10 mW/cm2), it gave an open circuit voltage of ~0.26V and a short circuit current ~1pA. Its photovoltaic performance is currently limited by the thin ITO layer and the low build-in electric field. Our study has shown a simple and useful platform for gaining insight into nanowire charge transport and collection properties. Fundamental studies of such nanowire device are important for improving the efficiency of future nanowire solar cells or photo detectors. The individual a-Si:H-MWCNT photo cell can also be used as a sensor in ultra low power electronic systems.

## Poster Board | 50

### Comparison of transparent conductive films of thermally purified and acid-purified single walled carbon nanotubes

**Seung Ho Lee**, *Faculty of Nanotechnology and Advanced Materials Engineering, Sejong University* | **Jeung Choon Goak**, *Faculty of Nanotechnology and Advanced Materials Engineering, Sejong University* | **Chung Yeol Lee**, *Faculty of Nanotechnology and Advanced Materials Engineering, Sejong University* | **Naesung Lee**, *Faculty of Nanotechnology and Advanced Materials Engineering, Sejong University*

Here, we studied on the transparent conductive films (TCFs) fabricated with as-produced SWCNTs and the SWCNTs subject to thermal purification and acid purification. The parameters contributing to the electrical conductivity of SWCNT networks mainly depend on purity, length and diameter of bundles, tube electronic type, doping, bundle-to-bundle contact, etc. The purification processes would affect some of these parameters, in particular, purity and length and diameter of bundles. The purity of SWCNTs was characterized by observing absorption peaks of the semiconducting (S22) and the metallic (M11) tubes in UV-Vis NIR spectroscopy and metal content in thermogravimetric analyzer (TGA). The samples containing different contents of SWCNTs were dispersed in water using sodium dodecylbenzensulfate (SDBS). The absorbances in the aqueous SWCNT suspensions were controlled to the almost same level to ensure the films having similar transmittances. SWCNT TCFs were formed by spraying the SWCNT suspension onto PET substrates. TCFs fabricated were evaluated in terms of the ratio of dc to optical conductivity for each film. The thermally purified SWCNT films showed higher ratios of dc to optical conductivity than acid-purified ones both before and after nitric acid treatment. It is expected that the conducting paths of SWCNT networks were increased due to smaller diameters and greater lengths of SWCNT bundles in the thermally purified SWCNT films although the purity of thermally purified SWCNTs were lower than that of the acid-purified one, as observed by using scanning electron microscopy and transmission electron microscopy.

## Poster Board | 80

### Saturation effects in (6,5) carbon nanotubes

**Jude R. Schneck**, *Departments of Chemistry and Physics and The Photonics Center, Boston University, USA* | **Andrew G. Walsh**, *Departments of Chemistry and Physics and The Photonics Center, Boston University, USA* | **Alexander A. Green**, *Department of Material Science and Engineering, Northwestern University, USA* | **Mark C. Hersam**, *Department of Material Science and Engineering, Northwestern University, USA* | **Lawrence D. Ziegler**, *Departments of Chemistry and Physics and The Photonics Center, Boston University, USA* | **Anna K. Swan**, *Departments of Chemistry and Physics and The Photonics Center & Department of of Electrical and Computer Engineering, Boston University, USA*

The nonlinear pump fluence dependence of the E22 transition of (6,5) carbon nanotubes at early delay times (~38 fs) was investigated via ultrafast pump probe spectroscopy over a pump fluence range of 1013 to ~1017 photons/cm-2. As pump fluence increases the pump-probe response saturates and at the highest fluence regimes the peak signal intensity decreases with increasing fluence. The signal was analyzed using third order perturbation theory for a two level system where the dephasing time, T2, is fluence dependent and is the only fitting parameter. Experimental values of the applied electric field along with the temporal profile of the pump and probe electric fields and all time histories in the probe detection direction were included in the data analysis. The material response is well fit by a fluence dependent dephasing model, $1/T2(NX)=1/T2^{1}+bNx$, where $T2^{1}$ = 58 fs and b = 7.2x10-5 µm/fs. Nx is the linear exciton density. Thus the nonlinear intensity dependence is largely attributed to exciton-exciton interactions on single carbon nanotubes.

## Poster Board | 82

### Dual Function of Double-Walled Carbon Nanotubes

**Morinobu Endo**, *Shinshu University*

Double-walled carbon nanotubes (DWNTs) have attracted lots of attention because their coaxial structures make them mechanically, thermally and structurally more stable than single-walled carbon nanotubes (SWNTs). Their intrinsic geometry allow inner SWNTs to exhibit exciting transport and structural properties that make them promising in the fabrication of field-effect transistors, stable field emitters and lithium ion batteries. In addition, selective modification of the outer tubes makes DWNTs useful for anchoring semiconducting quantum dots as well as for use as multi-functional filler in producing tough, conductive transparent polymer films, while the inner tubes with diameter below 0.9 nm preserve their excitonic transitions. In this talk, I have described the synthesis techniques of preparing highly pure and crystalline DWNTs with small inner diameters, their interesting optical and electronic properties in surfactant-dispersed DWNT suspensions, and, finally, the promising usages of DWNTs that have been developed in recent years.

## Poster Board | 85

### Ultrafast carbon nanotubes optical properties for high-bit-rate telecommunications applications

**Maud Gicquel-Guezo**, *FOTON, INSA (Rennes, France)*
**H. Nong**, *FOTON, INSA (Rennes, France)* | **M. Perrin**, *FOTON, INSA (Rennes, France)* | **C. Levallois**, *FOTON, INSA (Rennes, France)* | **F. Grillot**, *FOTON, INSA (Rennes, France)* | **S. Loualiche**, *FOTON, INSA (Rennes, France)* | **L. Bramerie**, *FOTON, ENSSAT ,France* | **A. Maalouff**, *FOTON, ENSSAT ,France* | **D. Bosc**, *FOTON, ENSSAT ,France* | **J.-C. Simon**, *FOTON, ENSSAT ,France* | **R. Fleurier**, *LEM (Châtillon, France)* | **B. L. Liang**, *Electrical Engineering Department (Los Angeles, USA)* | **D.L. Huffaker**, *Electrical Engineering Department (Los Angeles, USA)*

The quality of information transmission in telecommunications networks requires all-optical-regeneration of the optical signal, as it is damaged through its propagation in long-haul optical fibers. Our work focuses on designing efficient all-optical switches based on ultrafast and nonlinear optical properties of nanomaterials. We highlight here nonlinear optical properties of bundled carbon nanotubes (CNT), in direct comparison with quantum wells (QW): bundled CNT present ultrafast absorption dynamics and large 1D-excitonic nonlinearities. We aim at demonstrating the huge potential of bundled CNT-based optical devices for telecom applications[1], as simple-process and low-cost solution in comparison with QW-based devices [2]. Intrinsic properties of luminescent CNT are intensively investigated by international scientific community. Our study focuses more on CNT in bundles, where extrinsic properties govern optical properties. Thus, we preliminarily present linear optical properties of bundled CNT-films, in comparison with individualized luminescent CNT-films. Redshift and broadening of CNT optical transitions are clearly observed, from individualized to bundled CNT. Linear absorption in telecom window is also enhanced and we suggest the ability of bundled CNT-based devices to regenerate wavelength division multiplexing channels. Finally, nonlinear optical properties of bundled CNT-films are investigated using a femtosecond-pulses pump-probe experiment at 1550 nm. We compare the recorded dynamics of bundled CNT-films with QW. The subpicosecond recovery time of CNT-based devices should be suitable for a rate of telecom signal as high as 500 Gb/s. [1] H. Nong et al., Appl. Phys. Lett. (2010). [2] M. Gicquel-Guézo et al., Appl. Phys. Lett 85, 5926 (2004).

## Poster Board | 88

### Infrared Sensors Based on Multi-Wall Carbon Nanotube Films

**Philippe Mérel**, *Defence Research and Development Canada - Valcartier* | **Jean-Baptiste Anumu Keptsu**, *Plasmionique Inc.* | **Charlie Koechlin**, *Le centre français de recherche aérospatiale ONERA* | **Sylvain Maine**, *Le centre français de recherche aérospatiale ONERA* | **Riad Haidar**, *Le centre français de recherche aérospatiale ONERA* | **Jean-Luc Pelouard**, *Laboratoire de photonique et de nanostructures du CNRS* | **Andranik Sarkissian**, *Plasmionique Inc.* | **Ionescu Mihnea Ioan**, *University of Western Ontario* | **Xueliang Sun**, *University of Western Ontario* | **Philips Laou**, *Defence Research and Development Canada - Valcartier* | **Suzanne Paradis**, *Defence Research and Development Canada - Valcartier*

In order to fabricate novel infrared sensors, films of multi-wall carbon nanotubes have been grown on silicon and alumina substrates, using Plasma enhanced Chemical Vapor Deposition technique. The physical and optical characteristics of the devices were studied using variety of methods. To measure the infrared response of carbon nanotube based devices, two configurations were selected. In the first configuration, a perpendicular geometry, a Si/TiN/CNT/Au device was studied where the doped Si substrate and the 10 nm thick Au film were used as the electrical contacts. In the second case, a lateral geometry, two gold contacts were evaporated on the surface of the CNT film grown on an alumina substrate. The infrared response of both devices was measured and it was concluded that the detection behavior was consistent with those expected from bolometric effects. Measurements have also revealed a wide spectral response from the visible to 10 micrometer wavelength for both detectors. Optical characterization of the CNT films were also performed using infrared ellipsometry and the optical constants of the produced films were measured over wavelengths ranging from 0.4 to 15 micrometers.

## Poster Board | 93

### Position dependent photoconductivity in suspended single-walled carbon nanotube films

**Benoit St-Antoine**, *École Polytechnique de Montréal* | **David Ménard**, *École Polytechnique de Montréal* | **Richard Martel**, *Université de Montréal*

Over the last decade, numerous works have studied the photoconductivity in single-walled carbon nanotube films, both to answer fundamental questions about its driving mechanism as to assess its potential for practical applications (light detection, photovoltaic generation, etc.). [1,2] The origin of the photoconductivity is currently a matter of debate. Two opposing mechanisms have been proposed, i) a direct photoexcitation process or ii) a thermal effect. In this study, we have investigated the position dependent photovoltage of suspended single-walled carbon nanotube films in vacuum. The photoresponse of such films was found to be driven by a thermal mechanism, rather than by direct photoexcitation of carriers. [3] A model was developed to establish a relation between the photoresponse profile and the local Seebeck coefficient of the film, thus opening up new perspectives for material characterization. The technique was demonstrated by monitoring the doping changes in the nanotube films obtained by successive current conditioning steps. Since the Seebeck coefficient of carbon nanotubes spans a considerable range depending on their doping state, the photovoltage amplitude can be tuned and large responses have been measured (up to 0.75mV for 1.2mW). [1] A. Fujiwara et al. Jpn. J. Appl. Phys. Part 2-Lett. 40, L1229 (2001) [2] M. E. Itkis et al. Science 312, 413 (2006) [3] B. St-Antoine et al. Nano Lett. 9, 3503 (2009)

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### Energy transfer dynamics in functionnalized carbon nanotubes.

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Functionnalized NT are very promising materials for light harvesting applications since they combine the exceptional transport properties of carbon nanotubes and the versatility of organic dyes. In this study we show that a very strong interaction can be induced between porphyrin molecules and nanotubes, even in the context of non-covalent functionnalization. This interaction leads to very efficient energy transfer from the dye to the nanotube [1, 2]. We investigate its dynamics by means of broadband femtosecond transient spectroscopy. We show that the excitation of the porphyrin molecule is first followed by a internal energy conversion down to the Q band (~100fs), followed by a subpicosecond transfer to the nanotube. The population build up is observed on the lowest exciton level of the nanotube in agreement with photoluminescence measurements. Finally, we show that the quantum efficiency of this transfer can be very close to 1 with an almost total quenching of the porphyrin luminescence but a strong luminescence of the nanotube and with a strong acceleration of the relaxation in the donor. [1] G.Magadur et al ChemPhysChem 9, 1250 (2008) [2] C.Roquelet et al, http://arxiv.org/abs/0910.5619v1

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### Emission Saturation of Single-Wall Carbon Nanotubes via Modulation of Surfactant Interaction at the Nanotube Surface

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The optical properties of single-walled carbon nanotubes (SWNTs) offer great promises. However, the realization of their potential is limited by polydispersity and the degree to which the SWNTs are individually suspended and isolated from their immediate surroundings. The SWNT/surfactant hybrid undergoes a complex dynamic process that involves constant adsorption and desorption of surfactant molecules onto the SWNT surface; this dynamic process can be affected by the SWNT chirality, presence of electrolytes, and many other extrinsic factors which create changes in the adsorbate density around the tubes. This will, in turn, lead to changes in the emission properties of the SWNTs and alter the ability to separate SWNTs via DGU. In this work we study how addition of electrolytes affects SWNT/surfactant interactions. Electrolyte modulation via salt addition enhances the nanotube optical properties and the ability to achieve separation via DGU. More precisely, we show how surfactant concentration and addition of low concentrations of salt to individually suspended SWNTs in anionic surfactant effectively changes the SWNT/surfactant density; blushifting, narrowing, and enhancement of the absorbance and emission properties of SWNTs are observed. These optical changes are shown to be highly dependent on SWNT chirality with eventual aggregation at high salt addition. The manipulation of the SWNT/surfactant unit by controlled salt addition also improves the diameter-dependent separation of highly enriched metallic and semiconducting fractions. However these phenomena are not universal for all SWNT suspensions; the surfactant and/or surfactant mixtures must be optimized for ideal interactions with the chosen electrolyte.

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### Raman and Fluorescence Spectroscopic Studies of DNA-Dispersed Double Walled Carbon Nanotube Solution

**Jin Hee Kim**, *Shinshu University* | **Yoong Ahm Kim** | **Morinobu Endo** | **Mauricio Terrones** | **Mildred Dresselhaus**

Here we have carried out detailed Raman/luminescence spectroscopic studies on ssDNA-dispersed double walled carbon nanotubes (DWNTs) solutions at different dispersion states, in comparison with an SDBS-dispersed DWNT solution using three different laser lines, in order to understand the interactions between DNA and the outer tubes, and the effect of these different DWNT environments on the vibrational and luminescence behaviors. The luminescence peaks were intensified and shifted to longer wavelengths with the improved dispersion state of the DWNTs in an aqueous DNA solution, indicating that DWNTs are individually dispersed in an aqueous solution, which is strongly supported by the strong PL map and the sharp absorption spectra as well as high-resolution TEM observations. Noticeably, we observed cases of completely depressed RBM intensities associated with the outer tubes (regardless of their metallicity) for three configurations of DWNTs. This result strongly supports the interpretation that the evolved luminescence and sharp absorption peaks solely come from the semiconducting inner tubes of the DWNTs, not from impurity SWNTs. Conclusively, the circumferentially wrapped DNA on the outer tubes of individually isolated DWNTs in an aqueous solution gives rise to strong charge transfer to the semiconducting and metallic outer tubes as well as generating physical strain in the outer tubes. Therefore, we envisage that DNA-dispersed DWNTs are highly promising for producing strong and stable luminescence signals as well as for high yield optoelectronics applications.

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### Surfactant and structure-dependent exciton mobility in SWCNTs

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Exciton mobility in nanotubes is an intriguing phenomenon that plays a central role in nonlinear optical responses of single-walled carbon nanotubes (SWCNT) and results in the strong quenching sensitivity of SWCNT photoluminescence (PL) to covalent functionalization or oxidation. It was previously shown that single-molecule reactions of diazonium salts with individual SWCNTs can be observed as stepwise quenching of PL intensity. By analyzing the relative amplitudes of quenching steps, the range of exciton excursion along the nanotube during their lifetime was found be ~100 nm. In this study we describe a refined experimental methodology for quantifying exciton mobility of individual SWCNTs. We report exciton ranges of 140-240 nm in different environments that correlate weakly with PL intensity. These results are consistent with a model of localized SWCNT excitons having substantial mobility along the nanotube axis. An approximate proportionality was deduced between exciton range and the square root of excitonic lifetime indicating that exciton motion is diffusional and that it depends systematically on environment. However, exciton ranges measured for a variety of (n,m) structures indicate no substantial dependency on chirality, diameter and PL intensity.

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### Photophysics of polymer wrapped Single–Walled Carbon Nanotubes

**Jia Gao**, *University Of Groningen* | **Maria Antonietta Loi**, *University Of Groningen*

Recently, polyfluorene homo- and copolymers have proven to be very effective in the dispersion of single-walled carbon nanotubes (SWNTs), showing unique selectivity for a narrow distribution of semiconducting species [1,2]. The photophysical properties of such hybrids are extremely interesting because they offer the possibility to study the interaction between the polymer and SWNTs with minimal influence from metallic components. We report on the properties of poly (9,9-dioctylfluorenyl-2,7-diyl) (PFO)-wrapped SWNTs. We found that the photophysical properties of the dispersed SWNTs are strongly influenced by the solvent, the SWNT-polymer weight ratio and post- processing treatment [2]. Time-resolved photoluminescence measurements show a variation of the decay of (7,5) tubes from a few picoseconds to tens of picoseconds. It is rationalized that the difference is due to inter-tube exciton energy transfer from larger to smaller band gap tubes, and clearly such interaction became more efficient with the increase of the residual bundles in the dispersion. Moreover, by means of low temperature time-resolved photoluminescence measurements we gain a deep understanding of the dynamics of 'bright' excitons in semiconducting nanotubes.  [1] F. Chen, B. Wang, Y. Chen, L. -J. Li, Nano Letters. 2007, 7, 3013 [2] J. Gao, M. A. Loi, The European Physical Journal B-Condensed Matter. DOI: 10.1140/epjb/e2009-00420-0

## Poster Board | 116

### Optical properties and electronic structure of (6,5)/(6,4) single wall carbon nanotubes

**Thomas Pichler**, *University of Vienna* | **Katrien De Blauwe**, *University of Vienna* | **Duncan Mowbray**, *Donostia Science Center San Sebastian* | **Paola Ayala**, *University of Vienna* | **Ferenc Simon**, *University of Vienna* | **Angel Rubio**, *Donostia Science Center San Sebastian* | **Patrick Hoffman**, *Helmhotz Center Berlin* | **Hidetsugu Shiozawa**, *Surrey University* | **Yasumitsu Miyata**, *Nagoya University* | **Hans Kuzmany**, *University of Vienna* | **K Yanagi**, *Tokyo Metropolitan University* | **Hiromichi Kataura**, *AIST Tsukuba*

Due to the growing number of applications of small diameter single wall carbon nanotubes (SWCNTs) in opto- electronics and biological imaging, there is a strong need for better understanding their electronic properties. This presentation reports on a detailed analysis of the electronic structure of (6,5)/(6,4) nanotubes using high energy spectroscopy and optical techniques as probes. First the distribution and relative fraction of the two constituents are elucidated using optical, luminescence and resonance Raman spectroscopy. The details of the Resonance will be compared to the complementary resonance Raman response of (6,5),(6,4) inner tubes in DWCNT grown from ferrocene precursors with special emphasis to the influence of different van der Waals interactions. In the second part we will present the detailed valence and conduction band response of these narrow diameter tubes using x-ray absorption and photoemission as probes. For thick diameter tubes the results of these measurements allow a direct comparison to tight binding and ab-initio calculations. For the narrow diameter tubes these calculations are influenced by curvature effects giving rise to modified band structure and excitation spectrum. Here we compare the observed electronic structure and optical properties to recent ab-initio calculations. Work supported by the DFG projects PI 440 3/4/5 and FWF project P21333-N20.

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### Thermal light emission from suspended films and individual carbon nanotube transistors

**Elyse Adam**, *École Polytechnique de Montréal* | **Benoit Cardin St-Antoine**, *École Polytechnique de Montréal* | **Pierre Lévesque**, *Université de Montréal* | **David Ménard**, *École Polytechnique de Montréal* | **Richard Martel**, *Université de Montréal*

In the last few years, many papers reported on the light emission from electrically excited individual and network carbon nanotube transistors. Most of these works ascribed the emission to originate from electroluminescence. There are however a few reports on possible thermal contributions to the emission.[1-3] To clarify this question, we measured light emission spectra from two different types of CNT devices where thermal effects are expected in order to extract the spectral characteristics of the emission. The first type is a macroscopic suspended carbon nanotubes film where thermal radiation from Joule heating is expected. The second type is composed of individual carbon nanotube transistors deposited on a substrate and measured in vacuum. For both types of devices, an agreement between the Planck's formula and the spectra has been found at high bias. This indicates that the light emission at high bias arises mainly from heat. We compared these thermal spectra with typical electroluminescence spectra and extracted the main spectral signature from both regimes. While the thermal spectra follow the Planck's law, the electroluminescence spectra show a peak coming from excitonic recombinations. Both spectral signatures can be observed on the same devices by changing the operating conditions.  [1] Marty et al., Phys. Rev. Lett. 96, 136803 (2006) [2] Mann et al., Nat. Nano. 2, 33 (2007) [3] Lefebvre et al., Phys. Status Solidi RRL, 3, 199 (2009)

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### Exciton diffusion in air-suspended (9,8) carbon nanotubes

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Understanding of exciton dynamics in single-walled carbon nanotubes is essential for developing carbon-based nanoscale optoelectronics. In particular, diffusion of excitons governs the exciton-exciton annihilation process, which in turn determines the efficiency of optical emission from nanotubes. Here we report direct measurements of the diffusion length of excitons in air-suspended single-walled carbon nanotubes [arXiv:1003.0733]. Individual nanotubes are identified by photoluminescence imaging, while their lengths and chiral indices are determined by excitation spectroscopy and polarization measurements. With data obtained from 35 individual (9,8) carbon nanotubes, we are able to extract the exciton diffusion length by comparing the dependence of photoluminescence intensity on the nanotube length with numerical solutions of diffusion equations. We find that the diffusion length is at least 610 nm, which is substantially longer than those reported for micelle-encapsulated carbon nanotubes. The apparent diffusion length becomes shorter with higher excitation powers, consistent with exciton-exciton annihilation effects.

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### Influence of chirality and environment on the asymmetry of Raman resonance windows of individual single-walled carbon nanotubes

**Mario Hofmann**, *Massachusetts Institute Of Technology* | **Ya-Ping Hsieh**, *Massachusetts Institute Of Technology* | **Hootan Farhat**, *Massachusetts Institute Of Technology* | **Jing Kong**, *Massachusetts Institute Of Technology* | **Mildred Dresselhaus**, *Massachusetts Institute Of Technology* | **Ado Jorio**, *Universidade Federal de Minas Gerais* | **Marcos Pimenta**, *Universidade Federal de Minas Gerais* | **Martin Kalbac**, *J. Heyrovsky´ Institute of Physical Chemistry*

Resonance Raman excitation profiles of individual single-walled carbon nanotubes were investigated. An asymmetry in these profiles was observed that is related to different intensities of the involved resonant scattering processes. A chiral angle dependence of the asymmetry was found to be caused by variations in the defect density. Our analysis suggests that doping of the nanotube by adsorbates is the reason for changes to the resonance window shape. Consequently the resonance window width could be smaller than predicted and affected by environmental changes. Implications for nanotube metrology are discussed.

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### Non-Radiative Exciton Decay in Single-Walled Carbon Nanotubes

**Mark Harrah**, *Boston University* | **Anna Swan**, *Boston University*

Experiments have shown step-wise changes in the fluorescence intensity from single-walled carbon nanotubes[1,2]. It has been proposed that the underlying mechanism for the step-wise changes is diffusion-limited quenching of excitons at defects[1]. This property has been used to demonstrate single-molecule detection for biological applications[3]. We explore the role of defects on the quantum efficiency of nanotubes. We perform a Monte-Carlo simulation of the quantum efficiency using an exciton random-walk and defect-induced quenching model. The quantum efficiency is seen to depend only weakly on the number defects, but it is strongly related to the mean-square distance between defects. [1] Cognet, L. et al. Science 316, 1465-1468 (2007). [2] Jin, H. et al. Nano Lett. 8, 4299-4304 (2008). [3] Heller, D. A. et al. Nature Nanotech. 4, 114–120 (2009).

## Poster Board | 128

### Diffusion limited contact quenching of excitons in (6,5) SWNTs

**Tobias Hertel**, *University Of Würzburg* | **Sabine Himmelein**, *University Of Würzburg* | **Thomas Ackermann**, *University Of Würzburg* | **Dominik Stich**, *University Of Würzburg* | **Jared Crochet**, *University Of Würzburg*

Photoluminescence quantum yields and non-radiative decay of the excitonic S_1 state in length fractionated (6,5) single-wall carbon nanotubes (SWNTs) was studied by continuous wave and time-resolved fluorescence spectroscopy. We present a model for diffusion limited contact quenching of excitons at stationary quenching sites and tube ends. A combined analysis of time-resolved photoluminescence decay and the length dependence of quantum yields allows to determine average quenching site distances in our samples d_t=(120±25) nm, exciton diffusion lengths l_d=(210±40) nm, the exciton diffusion constant D=(10.7±0.4) cm^2s^-1, the long tube PL QY of 1.3% and the long tube PL lifetime of 20 ps.

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### Implementation of a Single Walled Carbon Nanotube-Enhanced Epoxy Solution for Crack Detection Applications

**Behnam Ashrafi**, *Institute for Aerospace Research-NRC* | **Yadienka Martinez-Rubi**, *Institute for Aerospace Research-NRC* | **Marcias Martinez**, *Steacie Institute for Molecular Sciences-NRC* | **Johnston Andrew**, *Institute for Aerospace Research-NRC* | **Benoit Simard**, *Steacie Institute for Molecular Sciences-NRC*

The success of Structural Health Monitoring (SHM) is typically limited by the availability of solutions for an accurate detection of a crack in both composite and metallic structures. The National Research Council Canada Institute for Aerospace Research (NRC-IAR) has been working on the development of a Surface Mountable Crack Detection System (SMCDS) for aerospace applications. The "intelligence" of the sensor is provided by a signal drop as the crack passes through a conductive paint layer. The SMCDS is limited in the amount of strain to which it can be subjected (typically below 3000 microstrain). Although sufficient for many applications, some fatigue experimental tests have demonstrated the need for sensors that can withstand higher strain levels (up to 6000 microstrain). This work focuses on the potential application of a SWCNT-modified epoxy as the conductive element of the SMCDS for higher strains. The primary objectives of adding SWCNT are to increase the epoxy electrical conductivity to a conductive regime suitable for SMCDS applications and to adjust mechanical properties of epoxy to withstand strains higher than 3000 microstrain. This work focuses on characterization of the mechanical and electrical properties of SWCNT/epoxy for this specific application.

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### Ultra-thin membranes of well-aligned single-walled carbon nanotubes

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Background An innovative, far-ranging application of carbon nanotubes is proposed: a study on microporosity instrumentation in cementitious materials has underlined the need for ultrasonic transducers with 1 µm size and 1 GHz operating frequency. Relying on previous demonstrations of single nanotube high-frequency vibration capabilities, an ultrasonic transducer device based on a vibrating membrane of aligned single-walled carbon nanotubes (SWNT) is being realized to meet these requirements [1]. Design and process To form the nano-membrane, SWNTs are densely aligned by dielectrophoresis, anchored with a metal ribbon and suspended over a trench, at the bottom of which lies the command electrode for the membrane electrostatic actuation. Results High resolution AFM imaging of the membranes proves their exceptionally low thickness, below 5 nm. SEM images, processed by a new method, quantitatively underline their high density and alignment rate. AFM force-distance curves yield the string constants of bundles of SWNTs composing the suspended membranes. An original data correlation method provides with an estimate of the SWNTs Young's modulus. Conclusion: Using SEM and multimode AFM imaging, we have proven suspension of our ultra-thin, rigid SWNTs membranes over 300 nm to 2 µm wide trenches. Their form factor, typically above 150, is considerably higher than the typical value of 50 in state-of-the-art ultrasonic microtransducers. Such performance is made possible by the high stiffness and form factor of SWNTs. [1] B. Lebental et al, "Capacitive ultrasonic micro-transducer based on a carbon nanotubes membrane", Proceedings of C2I10, January 2010, Le Mans, France

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### Manipulation of C60 Molecules by Electron Beam and Its Application to Attach Carbon Nanotubes to a Substrate

**Ryosuke Senga**, *Graduate School of Engineering, Osaka University; CREST, Japan Science and Technology Agency* | **Kaori Hirahara**, *Graduate School of Engineering, Osaka University; CREST, Japan Science and Technology Agency* | **Yoshikazu Nakayama**, *Graduate School of Engineering, Osaka University; CREST, Japan Science and Technology Agency*

The manipulation of nanosized materials is a key technology in the bottom-up fabrication of miniaturized devices. In this work, we have found that electron beam irradiation induces migration of C60 molecules from the outside toward the inside of the irradiation area. This is a manipulation of C60 molecules by using an electron beam. Thus we have applied this technology to attach carbon nanotubes (CNTs) to a silicon substrate. C60 molecules with a few molecular layers were deposited on a silicon substrate. The converged electron beam was brought close to the edge of the substrate coated with the C60-molecular layers in a transmission electron microscope. When the electron-beam intensity at the edge of the silicon substrate was ca. 6~10^6 electrons/nm^2, the C60 molecules migrated toward the center of the electron beam. The most possible driving force of the migration of C60 molecules is the Coulomb repulsion, which is caused by the negative charges induced to C60 molecules from the electron beam. For the application of the manipulation technology, a CNT was placed at the edge of the silicon substrate coated with the C60-molecular layers. Then, the converged electron beam was irradiated near the CNT. The C60 molecules continuously gathered to a central part of the irradiation area and covered a part of the CNT. The dose of electrons of 3~10^8 electrons/nm^2, moreover, changed the structure of the gathered C60 molecules to form a graphitic structure. This structural change functioned effectively to attach the CNT to the substrate.

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### Carbon Nanotube Probes : a new start ?

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Users of local probe methods such as Atomic Force Microscopy encounter every day tips related problems, such as a too large tip to obtain sufficient resolution or enter shallow holes, face tip wear or tip pollution that enlarge the tip and force the change of probe, a costly and time consuming burden. CNT as probes improve the mechanical and chemical stability together with a small size and a large aspect ratio. Spectacular demonstrations of carbon nanotube tips contributions have been published since 1996 on various samples,.. Despite the nanotube tips high intake, the use of such CNT tips hasn’t spread as much as expected. Two main reasons explain the limited development of CNTs: the difficult control of the nanotube length orientation and attachment to tip, and the complex mechanical nanotube behavior. With the latest synthesis progress and the large literature on nanotube tips specific properties, it may is time now for their development. Two strategies for nanotube tip fabrication will be presented : either direct growth of SWCNT by Hot Filament CVD on commercial tips, or synthesis of MWCNT on a filament followed by manual attachment to a tip. Examples of nanotube probes intakes will be given for imaging, but also other more exotic experiments where nanotube probes bring new solutions for nanoscale characterizations. In particular, we will see that there is something to do with long flexible tubes. Finally solutions for unique nanotube probe in situ charaterizations will be discussed.

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### Extremely high field emission performance of carbon nanotube emitters fabricated by new filtration-transfer technique

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There have been several methods to fabricate carbon nanotube (CNT) emitters, which include as-grown, spraying, screen-printing, electrophoresis and bonding methods. Unfortunately, these techniques generally suffer from two main problems. One is a weak mechanical adhesion between CNTs and the cathode. The as-grown, spraying and electrophoresis methods show a weak mechanical adhesion between CNTs and the cathodes, which induce CNT emitters pulled out under a high electric field. The other is a severe degradation of the CNT tip due to organic binders used in the fabrication process. The screen-printing method which is widely used to fabricate CNT emitters generally shows a critical degradation of CNT emitters caused by the organic binder. Such kinds of problems induce a short lifetime of the CNT field emitters which may limit their practical applications. Therefore, a robust CNT emitter which has the strong mechanical adhesion and no degradation is still a great challenge. We fabricated thin multi-walled CNT field emitters using a new filtration-transfer method. A very high emission current density of 500 mA/cm2 was achieved by CNT field emitters by using the method. We consider that the high emission current of the thin-MWCNT emitter using the filtration-transfer method may be attributed to the high density of emission sites at the CNT emitter, the good electrical contact, the strong mechanical adhesion between CNTs and the cathode, and the low degradation of CNT tips. It is suggested that the filtration-transfer technique is an effective way to realize organic binder-free, low-cost, large-size and high-performance CNT emitters.

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### Directed electrical energy release from Carbon Nanotube-Guided Thermopower Waves

**Wonjoon Choi**, *MIT, Chemical engineering department, USA; MIT, Mechanical engineering department, USA* | **Seunghyun Hong**, *Sungkyunkwan University, Mechanical engineering, South Korea* | **Joel Abrahamson**, *MIT, Chemical engineering department, USA* | **Jaehee Han**, *MIT, Chemical engineering department, USA* | **Changsik Song**, *MIT, Chemical engineering department, USA* | **Nitish Nair**, *MIT, Chemical engineering department, USA* | **Seunghyun Baik**, *Sungkyunkwan University, Mechanical engineering, South Korea* | **Michael Strano**, *MIT, Chemical engineering department, USA*

Theoretical calculations predict that by coupling an exothermic chemical reaction with a nanotube or nanowire possessing a high axial thermal conductivity, a self-propagating reactive wave can be driven along its length. Herein, such waves are realized using a 7-nm cyclotrimethylene-trinitramine annular shell around a multi-walled carbon nanotube and are amplified by more than 104 times the bulk value, propagating more than 2 m/s, with an effective thermal conductivity of 1.28 kW/m/K at 2860 K. This wave produces a concomitant electrical pulse of disproportionately high specific power, as large as 7 kW/kg, that we identify as a thermopower wave. Thermally excited carriers flow in the direction of the propagating reaction with specific power that scales inversely with system size. The reaction also evolves an anisotropic pressure wave of high total impulse per mass (300 N-s/kg). Such waves of high power density may find uses as unique energy sources.

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### Anisotropic carbon nanotube products fabricated with carbon nanotube web

**Yoku Inoue**, *Shizuoka University* | **Akihiro Ishida**, *Shizuoka University* | **Morihiro Okada**, *Shizuoka University* | **Hidenori Mimura**, *Shizuoka University*

Multi-walled carbon nanotube (MWNT) arrays were synthesized using a conventional thermal chemical vapor deposition (CVD) system. As a precursor of Fe catalyst, FeCl2 powder was loaded into the growth chamber with a Si or SiO2 substrate. To grow MWNT arrays, single acetylene gas was flown. Densely grown MWNTs are vertically aligned on a quartz substrate, and show a high drawable feature. The drawn MWNT web was easily drawn by pinching and pulling the array edge. To date the grown 2.5 mm-long array is drawable. The web is very sticky, and so it is easily fabricated into large scale nanotube products, including a MWNT fiber and a sheet. Since MWNTs are completely aligned in the drawn direction in the web, the fibers and sheets also have anisotropic properties. Electrical conductance is 2.5 times greater in the aligned direction than in the crossing direction. Needles to say, mechanical strength is much higher in the aligned direction. We will discuss about the growth of well-drawable MWNT array, drawing (spinning) the web, and building the anisotropic MWNT products, including detailed electrical and mechanical properties.

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### Carbon nanotube resonator in liquid

**Shunichi Sawano**, *Osaka Prefecture University* | **Takayuki Arie**, *Osaka Prefecture University; CREST-JST* | **Seiji Akita**, *Osaka Prefecture University; CREST-JST*

Carbon nanotube (CNT) resonator is anticipated as ultrasensitive detectors for measurement of mass and interactions of biological molecules. To achieve mass measurement of biological materials in viscous fluids using the CNT resonator we investigated the vibration of CNT cantilevers in water using the optical detection technique. To clarify the size limitation of the analysis based on the continuum theory, we first performed molecular dynamics simulations. In the simulation, even for the single wall nanotubes (5, 5) with the diameter of 0.7 nm, the continuum theory is applicable to nanotube vibrations. The diameter and length of typical CNT used in this study were 60 nm and 13.8 μm, respectively. In vacuum, we often found a few resonance modes (such as fundamental and second harmonic oscillation) of CNT vibrations. We then measured the resonant frequency of CNT vibration of the second harmonic oscillation in water. Note that the fundamental oscillation of the CNT often disappeared once the CNT was immersed in water. This was inevitable since lower modes of oscillation are more strongly affected by the viscosity of fluids. The resonant frequency of the CNT in water decreased with lowering the water temperature (the resonant frequency of 543kHz at 28.9°C decreased to 500kHz at 18.2°C) corresponding to the natural phenomenon by which liquid viscosity tends to increase at lower temperatures. This may imply that the CNT cantilever is also applicable to the local viscosity sensor of surrounding media.

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### Single-walled carbon nanotube film grown in-situ by induction thermal plasma: toward low cost highly sensitive pressure sensors

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Since the discovery of single-walled carbon nanotubes (SWCNTs), their incorporation into various materials has been proposed for a variety of areas. This extensive interest in developing SWCNTs applications is mainly attributed to their astonishing mechanical and electrical properties. Here, we report the fabrication of simple pressure sensors made from multi-layered SWCNT sheets grown in situ by induction thermal plasma. For comparison purposes, a regular SWCNT film, or “buckypaper”, was fabricated by vacuum filtering a purified suspension made from the as-grown SWCNT sheets. Scanning electron microscopy observations showed that the multi-layer sheets are composed of lightly woven nanotube bundles interlinked with amorphous carbon and catalysts particles while the regular SWCNT films demonstrated a denser structure almost perfectly exempt of impurities. We measured gage factors at least 50 times higher for the as-grown material, in comparison with the regular SWCNT film, and a significantly superior dynamic range. Two piezoresistive models were evaluated for describing the behavior of these simple sensors. The first one was based on the conduction mechanisms in conductor loaded composites while the other was based on the packing mechanics of fibre wads. Because of their low manufacturing cost and their high sensitivity, these as-grown SWCNT sheets would be ideal for the fabrication of large-size sensors.

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### Observation of Dynamic Strain Hardening in Polymer Nanocomposites

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Most materials respond either elastically or inelastically to applied stress, though degradation and premature failure may occur if repeated loading is great enough to induce structural fatigue. The cyclic compressive loading of vertically-aligned carbon nanotube/poly(dimethylsiloxane) nanocomposites has revealed an active strengthening mechanism not observed in the neat polymer, resulting in a discernable increase in stiffness which will continue for as long as dynamic stress is maintained and will begin again if dynamic stress is removed and reapplied. The nanotube alignment in samples allowed for orientation-specific measurement, and the behavior was amplified under compression transverse to the nanotube surfaces, implying that interfacial pressure catalyzes the change. Static stress showed no stiffening, and the above observations in conjunction with thermal analysis suggest that dynamic-stress-induced polymer chain alignment and/or curing at the interface are possible mechanisms for this self-strengthening behavior. Further understanding and exploitation of the mechanism(s) responsible for this strengthening may offer the potential for the development of robust self-strengthening materials. Control over the mechanism occurring here may also contribute to the pursuit of advanced polymer nanocomposites by further resolving nanoparticle/polymer interaction and facilitating the improvement of bulk mechanical properties via enhanced interfacial load transfer.

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### The mechanical and electrical properties of a single multi walled carbon nanotubes inside scanning electron microscope

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The mechanical and electrical properties of a single multi walled carbon nanotubes (MWCNTs) were investigated inside a scanning electron microscope. The mechanical strain was applied to the MWCNT by a tungsten tip controlled by a nano-manipulator. The load response during the tensile test for the MWCNT was obtained using the force sensor which was typed with cantilever. The fractured area of the MWCNT was observed by transmission electron microscope after tensile test. The tensile strength of the MWCNT was about 41.01 GPa and the elastic modulus was calculated at 0.98 TPa. The contact resistance between a single MWCNT and the tungsten tip decreased with the addition of carbon deposition during e-beam exposure. The electrical resistance was significantly changed during the elongation process of the MWCNT and corresponded with the nanotube strain. The strain sensitivity of a single MWCNT was calculated to be around 25. And also, we performed the field emission for a single MWCNT. The current-voltage characteristics of MWCNT during field emission were investigated by in-situ imaging and field emission measurement. The field emission from a single MWCNT follows Fowler-Nordheim behavior with a single linear slope in the plot.

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### Electron Spin Resonance in Oxygen-Free Single-Walled Carbon Nanotubes

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Previous electron spin resonance (ESR) studies of single-walled carbon nanotubes (SWNTs) have revealed various sample-related issues and problems, which resulted in an array of conflicting results and interpretations. Here we have performed temperature-dependent ESR measurements on compacted acid-purified laser-oven powder SWNTs before and after removing oxygen via annealing in argon. By compressing the SWNTs, we were able to produce a sample which circumvented many of the problems of previous studies. Removal of oxygen from the sample resulted in an increase of the ESR signal intensity by roughly two orders of magnitude, making it larger than the ferromagnetic resonance signal from remaining catalyst particles. This large SWNT resonance allowed us to study the ESR lineshape in unprecedented detail as a function of temperature and microwave power. The observed spectra are fit well by a modified Dysonian lineshape at all temperatures, suggesting electron delocalization. However, the spin susceptibility is found to increase with decreasing temperature, both in the as-prepared and oxygen-free SWNTs, indicating localization at low temperatures. Despite this trend, the temperature behavior of the susceptibility does not exhibit a Curie law. Furthermore, through the temperature dependence of the ESR lineshape, linewidth, and conductivity, we demonstrate quasi-one-dimensional variable range hopping between nanotubes in the oxygen-free sample. Specifically, careful fitting of the linewidth produces an unambiguous motional narrowing at elevated temperatures, providing an estimate for the inter-nanotube hopping frequency. Finally, we observe microwave-power-dependent asymmetry in the Dysonian lineshape, from which we expect to deduce the spin lifetimes of conducting, quasi-one-dimensional electrons.

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### Nitrogen-doped carbon nanotubes for catalytic reaction

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Nitrogen atoms entering in the graphene sheets as substitute of carbon could modify in a large extent the acido-basic properties and also surface adsorption properties of the nanotube and finally, the active phase anchorage and dispersion. This work reports the synthesis of aligned and entangled nitrogen-doped carbon nanotubes (N-CNTs) using a Chemical Vapor Deposition (CVD) and their subsequence use as catalyst support. Several characterizations, i.e. XPS, SEM and TEM were done on the as-synthesized N-CNTs in order to get more insight about the influence of the synthesis conditions on their physical and chemical properties. Depending on the synthesis conditions, the atomic percentage of nitrogen in carbon nanotubes varied from 1 to about 5.5 at. %. The activity of N-CNTs and undoped CNTs (N-free CNTs) for different reactions like hydrogenation of cinnemaldehyde and C-C cross-coupling reaction were studied in order to stress the advantage of doping of CNTs for their subsequent use as catalyst support. The introduction of nitrogen atoms into the carbon matrix significantly modified the chemical properties of the support compared to the N-free carbon nanotube resulted in a higher metal dispersion. N- CNTs exhibit much higher activity in the hydrogenation reaction compare to the undoped ones. Nitrogen incorporations also strongly improves the selectivity towards the C=C bond hydrogenation. The results also show that the nature of the nitrogen species incorporated into the CNTs structure drastically influenced the catalytic activity.

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### Density x diameter relationship of carbon nanotubes sorted in density gradients

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As-synthesized single-walled carbon nanotubes (SWNT) have been shown to be composed of heterogeneous bundles containing tubes of varying diameters and electronic structures. Recently a nondestructive sorting method was proposed in which nanotube bundles are dispersed in water-surfactant solutions and subsequently submitted to ultracentrifugation in a density gradient. Thus, SWNTs of different diameters are distributed according to their densities along the centrifuge tube. The best performance in discriminating nanotubes by diameter is obtained through a mixture of two anionic amphiphiles, sodium dodecylsulfate (SDS) and sodium cholate (SC). Surprisingly, small diameter nanotubes are found in the low density part of the centrifuge tube. In this work we study the water-surfactant-SWNT system using molecular dynamics simulations, which reveal that the surfactants can actually be attracted to the nanotube interior. The binding energy of the amphiphiles with SWNT depends weakly on diameter when they attach to the outer nanotube surface. Inside the tubes, on the contrary, the biding energy is strongly dependent on tube diameter and surfactant size: SDS fits best inside tubes from 8 to 9 Å in diameter, while SC has strongest binding in tubes of diameters from 10.5 to 12 Å. Molecular dynamics at room temperature shows that amphiphiles can drag water molecules along to the tube cage interior, promoting nanotube filling with both water and surfactant molecules. The resulting densities of filled SWNT and its variation with tube diameter are in agreement with experimental data.

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### Evaluation of the quality of a sorting of carbon nanotubes by density gradient ultracentrifugation

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As-synthesized samples of single wall carbon nanotubes are known to vary in chirality. They contain a mixture of metallic and semi-conducting carbon nanotubes. This heterogeneity prevents their use for the development of complex optical or electronic devices. Recently, Arnold et al. reported on the sorting of carbon nanotubes using density gradient ultracentrifugation (DGU) by enhancing the mass difference between nanotubes by a specific adsorption of surfactants. In this communication, we study the sorting of carbon nanotubes according to their electronic properties and their number of walls by using the DGU. We show how the efficiency of this method can be estimated in quantitative manner, by coupling TEM imaging and structural analysis and various spectroscopic measurements, namely optical absorption, Raman spectroscopy, and photoluminescence. Using these tools, we demonstrate that a high sorting quality, according to the metallic-semiconductor character, can be obtained by DGU for both single wall nanotubes and double-walled carbon nanotubes, by applying a two-step procedure. The first step consists in sorting semiconducting tubes. In the second step, the sorted fractions were reinserted and DGU was carried out under conditions which allow to sort metallic carbon nanotubes to a high extend. Applying this procedure, the content of metallic carbon single wall nanotubes could be reduced to 11% starting from an original value of 38 % and samples containing more than 90% of semi-conducting double wall nanotubes could be obtained.

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### N-type doping effect of Single Walled Carbon Nanotubes with aromatic amines

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We investigated the chemical doping of SWNTs networks by a treatment with aromatic amines. Adsorption and intercalation of amine molecules in bundled SWNTs leads to the typical n-type doping observed already for alkali metals. The electron donation to SWNTs is demonstrated by the XPS spectra, where the carbon C 1s peak observed at 284.4 eV for the sp2 carbon in pristine sample is shifted by 0.4 eV to higher binding energy upon chemical treatment. The development of a Breit-Wigner-Fano (BWF) component on the lower energy side of the G-mode in the Raman spectrum provides an evidence of the charge accumulation in the nanotube network. Thereby the shift of the Raman-active tangential vibration G mode by up to 12 cm-1 to lower frequency reflects the phonon softening and demonstrates a further evidence for the Fermi level shift in SWNTs. The spectroscopic changes are accompanied by the modification of SWNTs electrical properties. Reduction of electrical conductivity upon interaction with amine molecules is an indication for the electron transfer and decreasing the charge concentration in the naturally p-type doped semiconducting tubes. Among the two selected n-type dopants, the N,N,N',N'-tetramethyl-p-phenylene-diamine with two sp3 hybridized nitrogen atoms, shows stronger doping effect than the tetramethylpyrazine, where the nitrogen lone pairs are localized on the sp2 orbitals.

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### The effects of sonication on the degree of dispersion of carbon nanotubes in epoxy systems

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Epoxy systems filled with multiwall carbon nanotubes (MWNT) have been studied. It is generally believed that nanotubes must be well dispersed as single tubes in the matrix to utilize their excellent mechanical properties. Bath or tip sonicators are usually employed for the dispersion of the MWNTs. A bath sonicator treats the sample homogenously, but the power and the intensity is low. This results in very long sonication times to reach acceptable dispersions. Tip sonicators on the other hand, can have a high power output, but the acoustic field is very inhomogeneous. For larger volumes, stirring of the solution is necessary. Alternatively, the sonication can be done inside a flow-cell, resulting in a more homogenous sonication and a better ability to handle larger sample volumes. The efficiency of a bath sonicator has been compared with a tip sonicator in a flow-cell. Different types of MWNTs were dispersed in an epoxy curing agent. The degree of dispersion was determined by differential sedimentation particle analysis using a disc centrifuge. The results show that the particle size distribution is bi-modal with a narrow distribution of dispersed nanotubes and a broader distribution of agglomerates ranging from 100 nm to several micrometers in size. Furthermore, the separation of MWNTs from these agglomerates is controlled by a more complex mechanism than the energy input alone. At comparable energy inputs, a better dispersion is achieved using a higher acoustic intensity. The rate and degree of dispersion varies with different types of MWNTs.

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### Carbon nanotubes as platforms for electrochemical and electronic detection of biorecognition processes

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Carbon nanotubes have been exploited to reveal fundamental physical phenomena and to design novel nanodevices for a wide range of applications. For instance, the prominent electrochemical properties of carbon nanotubes have impelled the design of diverse electrode configurations. That combined with their chemical properties and (bio)functionalization versatility have made these materials very appropriate for the development of electrochemical biosensors. On the other hand, the semiconductor character of the nanotubes has been exploited for applications mainly in nanoelectronics and sensor technology by using a field effect transistor configuration with the nanotube acting as conductive channel. These types of devices turn out to be highly promising for biomolecule sensing and for the monitoring of biological processes. Under this context, the determination of specific DNA sequences is becoming an important diagnostic tool for many clinical and therapeutic applications. Various approaches for simple, fast, and sensitive specific detection of DNA sequences have been developed and improved during the last few decades. In this communication, we will overview different strategies for electrochemical or electronic detection of DNA sequences based on CNT nanotube modified devices. In the case of the electrochemical approach, CNT microelectrode arrays covalently functionalized with specific DNA probes have been used. The DNA target detection was monitored by using the cyclic voltammetry, chronocolometry or impedance measurements. On the other hand the electronic detection of DNA sequences was pursued by using carbon nanotube field effect transistors operating in liquid environment and by the use of bifunctional linkers for the immbolization of the DNA probe.

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### Enrichment of Armchair Carbon Nanotubes via Density Gradient Ultracentrifugation: Full Population Analysis using Raman Excitation Profiles

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Using resonant Raman scattering spectra collected over a broad range of excitation wavelengths (440-850 nm), we have constructed Raman excitation profiles of the radial breathing mode phonon for each (n,m) species present in as-produced and metal-enriched single-walled carbon nanotube ensemble samples. From this, we determine the relative abundances of all metallic and semiconducting chiralities. Strikingly, the data clearly show that our density gradient ultracentrifugation (DGU) process enriches the metal-enriched sample in armchair and near-armchair species. In particular, we observe that armchair carbon nanotubes constitute more than 50% of each metallic (2n + m) family yet observe little to no chiral angle dependence in the remaining semiconducting species minority. Such data combined with absorption and photoluminescence measurements elucidate elements of the mechanism of the DGU metallic type-enrichment process and the importance of surfactant micelle composition. Finally, we compare our measured relative abundances determined from Raman spectroscopy to absorption area estimates to assess the validity of the usage of absorption spectroscopy for determining % metallicity of ensemble nanotube samples.

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### Molecular dynamics simulation of ternary O2/N2/CO2 mixture flow in single-wall carbon nanotubes

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Gas adsorption and transport in carbon nanotubes (CNTs) are being investigated. A specific feature of CNTs is their adsorption selectivity, which should eventually be used for separation membranes. So far, theoretical studies of gas-mixture behaviour in CNTs deal mostly with binary mixtures. Non-equilibrium molecular dynamics simulations of the flow of a ternary O2/N2/CO2 mixture through single-wall open-ended CNTs are presented. Gas molecules are modelled as spherical particles, with all interactions modelled via the Lennard-Jones potential. The interaction potentials between different gas components, as well as between gas molecules and carbon atoms, are defined using the Lorentz-Berthelot combining rules. The chemical potential of individual components is evaluated using Widom's test particle method. The following different armchair nanotubes are considered: (10,10), (16,16) and (24,24), with diameters equal to 1.356 nm, 2.170 nm and 3.255 nm, respectively. Nanotubes are treated as rigid, and gas-nanotube potentials are summed-up over pair-wise contributions between gas molecules and each atom forming the nanotube. In the presented simulations, so-called room temperature was assumed (298 K), whereas the initial pressure in the carbon nanotubes was 1 bar. Equilibrium configurations were first established in the nanotubes by performing Grand Canonical Monte Carlo simulations. The equilibration process implicitly simulated gas adsorption on the nanotube walls. Then, the flow of the mixture was started by connecting a reservoir with a higher molecular density to the tube entrance. The ensuing flow rate through the nanotube was observed and the separation of gas mixture components during the flow was analysed.

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### An new combined protocol for large scale purification of SWNTs from arc discharge produced cloth-like soot

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Though the purification of single-walled carbon nanotubes (SWNTs) has been studied for more than ten years, it is still necessary to develop facile and efficient purification strategies for obtaining high-purity SWNTs on a large scale. In this study, high purity SWNTs is acquired from arc discharge produced cloth-like soot via a new purification protocol, namely gram scale of dirty SWNT felt are sequentially treated by HNO3/HCl refluxing, freeze-drying, steam treatment and HCl dissolution. Finally a product of >98% purity can be obtained with an overall yield of ~75% of the SWNTs in the raw soot. Various techniques like TGA, HRTEM-SEM, Raman and Vis-NIR spectroscopy, as well as magnetometry are employed to characterize the purity of the samples during the purification processes. A high IG/ID value 78.92 and a high relative purity 170.4% are achieved. In addition, the mechanical property of a buckypaper made of the purified SWNTs is evaluated. In-depth studies on the function and mechanism of each purification step are presented. And the results indicate that HNO3/HCl refluxing combined with freeze-drying is the key process that renders the oxidized SWCNTs soot hydrophilic along with a large surface area, and thus remarkably increases the efficiency of the steam treatment to remove most of the carbonaceous impurities. Furthermore, by experimental trails, we propose that this protocol can also be applied to the purification of double walled carbon nanotubes synthesized by arc discharge.

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### Gas-phase methodologies for the grafting and characterisation of carbon nanotube surfaces

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This paper aims to contribute to the understanding and control of carbon nanotube surface properties which are of great relevance for the processing of CNT materials and their performance in a broad range of applications, including composites, catalyst supports and sensing devices. We explore a generic, thermochemical furnace treatment that allows the introduction of a wide variety of functional species onto the CNT surface whilst maintaining the excellent properties of the untreated materials. The reaction is extremely versatile and can be applied entirely in the gas-phase, greatly simplifying work-up and improving scalability. The underlying reaction mechanism has been established and the distribution of the functionalised sites has been studied at the microscopic scale using tagging reactions. The effect of the treatments has also been characterised by various analytical techniques, such as thermal analysis (TGA), Raman spectroscopy and inverse gas chromatography (IGC). The application of IGC to carbon nanotubes has required significant development, but provides a new means to probe the nature of modified nanotube surfaces and extract important thermodynamic surface parameters, including surface energies, electron accepting and donating capabilities and adsorption capacities, which are difficult to obtain with other characterisation techniques. IGC results, dispersion studies and direct wetting experiments on the nanoscale have been used to assess and predict the interfacial compatibility of various modified CNTs with a broad range of media.

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### Raman spectroscopy of functionalized nanotubes

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The functionalization of carbon nanotubes with different chemical moieties is an efficient route to controlling solvent dispersion, electronic doping, electronic separation or molecule-nanotube binding energies. The attachment of molecular groups to the nanotube side-wall and its influence on the nanotube electronic structure has been subject of large interest to the nanotube research in the last years. Different effects on the electronic and vibrational properties are expected when the functional group is bound covalently or noncovalently to the nanotube surface, however, a direct evidence of how a chemical moiety modifies or modulates the nanotube electronic structure is still an open question. In this work we present a systematic study by resonant Raman spectroscopy of single-wall nantubes functionalized with different chemical groups and by different functionalization routes. Dependence of the functionalization with nanotube diameter and/or electronic character (semiconducting or metallic) has been investigated. Effects of the functional groups on the nanotube electronic and phonons structures are discussed.

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### Direct polymer grafting on carbon nanotubes by means of photopolymerization

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In spite of many attempts to obtain carbon nanotube (CNT)/polymer composite materials with extraordinary mechanical and electrical properties, the effective incorporation of CNTs within the surrounding matrix is still challenging. The reason is that, due to effective van der Waals attraction, CNTs form large agglomerates, known to behave differently from individual CNTs. Direct chemical modification of CNTs with polymer grafts proved to be efficient to enhance their dispersion ability, since long polymer chains can help to destroy the bundles of CNTs and prevent their subsequent self-agglomeration. We use self-initiated photografting and photopolymerization to form stable polymer grafts from vinyl monomers. The procedure is found to be successful for the functionalization of single- and multi-walled CNTs with polystyrene and poly(4-vinylpyridine). Raman spectroscopy and thermo-gravimetric analysis, applied for the characterization of the native and modified CNTs, show the dependence of the grafting density on time of polymerization. AFM images confirm efficient deagglomeration of the CNTs after the modification. SANS experiments (D11 at ILL) were performed in order to determine the dimensions of the native and modified CNTs and their behavior in solutions. CNTs modified with polymer grafts will be incorporated into suitable bulk block copolymers. Depending on the coating, the modified CNTs will accumulate in one of the polymer phases of the block copolymer. In this way, the block copolymer morphology will serve as a three dimensional template for the directed assembly of the modified CNTs.

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### The effect of barrier layer-mediated catalytic deactivation in vertically aligned carbon nanotube growth

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The effect of Al-barrier layer-mediated Fe-catalytic deactivation in vertically aligned carbon nanotube (CNT) growth were studied. The substrate surface morphology, catalytic diffusion and barrier layer oxidation were found to be dependent on the annealing temperature of the barrier layer, which ultimately affects CNT growth. The annealed barrier layer without complete oxidation was found to be suitable for top to bottom super aligned CNT arrays. The highest average CNT growth rate of up to 3.88 µm/s was observed using this simple approach. Details of the analysis are also presented.

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### The Initial Stages of SWCNT CVD Synthesis on SiO2 Nanoparticles: A QM/MD Investigation

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The ability of non-metal catalysts, notably SiO2, to assist the nucleation and growth of SWCNTs via CVD has recently been established [1]. Speculations that the traditional VLS mechanism is possibly responsible for SWCNT nucleation on silica nanoparticles have also been made recently [2]. However, the exact mechanism by which SiO2 assists the nucleation and growth of SWCNTs remains unknown. In this work, we address this issue by simulating CH4 CVD on a SiO2 nanoparticle at 1200 K using QM/MD simulations. In contrast to CVD using traditional Fe-group catalysts, CVD on SiO2 induced a complex chemical process. Most notably, CO was produced as the primary chemical product via the carbothermal reduction of SiO2, a fact that is consistent with recent experimental observations [2]. Ultimately, the insertion of carbon into/removal of oxygen from the SiO2 nanoparticle resulted in the local formation of amorphous SiC. However, this carbothermal reduction was limited to the outer regions of the catalyst, with the core of the particle remaining predominantly composed of Si and O. On this basis, we suggest that a traditional VLS model of SiO2-catalyzed SWCNT nucleation may by inadequate. The formation of a SWCNT "nucleus" on the SiO2 surface was ultimately observed following further annealing at 1200 K. Interestingly, components of this mechanism are reminiscent of those found during Fe-catalyzed SWCNT nucleation [3]. [1] Y. Homma et al., Nano Res., 2009, 2, 793. [2] A. Bachmatiuk et al., ACS Nano, 2009, 3, 4098. [3] Y. Ohta, et al., ACS Nano 2009, 3, 3413.

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### Lattice-oriented growth of single-walled carbon nanotubes applied to nanoscale lithgraphy

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Electron beam lithography is very powerful method for manufacturing integrated circuits and creating nanotechnology devices. And it is the highest resolution patterning method until the present. However, the key limitation of electron beam lithography is the time of process and throughput. Even if it is possible to pattern structure at 10 nm or below, it is expensive and time-consuming. Therefore attempts to improve its capability were performed for many years. Here, we present a new patterning technique of nanometer-wide metal lines. This technique is applied to the preparation of thin catalyst lines for the synthesis of single-walled carbon nanotubes (SWCNTs). First, we synthesize SWCNTs on ST-cut quartz substrate by Catalytic Chemical Vapor Deposition (CCVD). The CNTs can be grown with same direction which exactly followed by the X-axis of the quartz substrate. We studied the influence of the CCVD conditions on the density, diameter and length of the SWCNTs, because these determine the resolution and structure of the patterned metal lines. Then, we deposited metal (iron) directly onto these substrates having aligned nanotubes. Theses nanotubes with newly deposited catalyst were transferred onto SiO2/Si wafer. Wet etching by KOH was used to remove the metal directly lying on the SiO2 surface. In other words, initially synthesized nanotubes act as a metal supporter and a nanolithography template. These samples were subjected to a second CCVD growth and analyzed by FE-SEM, AFM, TEM and Raman spectroscopy.

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### Synthesis of N-doped carbon nanotube arrays

**PengXiang Hou**, *Institute Of Metal Research, Chinese Academy Of Sciences* | **Chang Liu**, *Institute Of Metal Research, Chinese Academy Of Sciences* | **HuiMing Cheng**, *Institute Of Metal Research, Chinese Academy Of Sciences*

N-doped carbon nanotubes (CNT) arrays were directly synthesized on a substrate in a 2-in. quartz tube reactor horizontally inserted into a tube furnace using a chemical vapor deposition method. The carbon and nitrogen source used is acetonitrile. The catalyst used is ferrocene. In a typical experiment, the furnace is heated to a fixed temperature under a gas flow of 500 sccm Ar and 100 sccm H2. Then, the mixed ferrocene/acetonitrile is added to the reactor using a syringe pump (as shown in Fig.2) at a controlled rate. The N-doped CNT arrays started to grow on the substrate put in the furnace. After the growth, the supply of the ferrocene/acetonitrile mixture is stopped and the furnace is cooled down to room temperature. The morphology, composition, and micro-structure of N-doped CNT arrays were characterized with scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive X-ray (EDX) analysis.

## Poster Board | 268

### Centimeter-Tall Carbon Nanotubes by Continuous Root Growth

**SangWook Park**, *Department of Chemical System Engineering, The University of Tokyo* | **Kei Hasegawa**, *Department of Chemical System Engineering, The University of Tokyo* | **Hisashi Sugime**, *Department of Chemical System Engineering, The University of Tokyo* | **Suguru Noda**, *Department of Chemical System Engineering, The University of Tokyo; PRESTO, Japan Science and Technology Agency*

Synthetic methods of carbon nanotubes (CNTs) need to be further developed to realize their possible applications. Millimeter-tall vertically aligned single-walled CNTs (VA-SWCNT) were achieved by the water-assisted chemical vapor deposition (CVD) on catalyst-supported substrates [1], however, CNT growth terminates in the end. Supplying ferrocene vapor during CVD enabled the continuous CNT growth on substrates with predeposited Fe catalysts, and yielded about 3-mm-tall VA-CNTs in 1 hour [2]. However, in conventional hot-wall CVD, Fe particles forming on CNT layers from ferrocene continuously nucleate additional CNTs, resulting in stacked CNT layers [3]. To obtain long and strong CNT wires, CNTs need to be grown continuously without additional CNT nucleation. We have previously developed a hot-wall CVD method yielding millimeter-tall VA-SWCNTs in 10 min [4] and a 'cold-gas' CVD method yielding such growth on selectively heated ribbon-shaped substrates while keeping the gas and CNTs unheated [5]. This time we applied the ferrocene supply to the cold-gas CVD to supply ferrocene and C2H2 efficiently to the catalysts on substrates from the side of VA-CNTs and confine their growth only at their roots. 2-cm-tall VA-CNTs were obtained in 12 h and the mechanism for prolonged CNT growth will be discussed. References: [1] K. Hata, et al., Science 306, 1362 (2004). [2] G. Eres, et al., Appl. Phys. Lett. 84, 1759 (2004). [3] Z. Yang, et al., Nanotechnology 19, 085606 (2008). [4] S. Noda, et al., Jpn. J. Appl. Phy. 46, L399 (2007). [5] R. Ito, et al., MRS Spring Meeting, P4.26, Mar. 2008.

## Poster Board | 270

### Horizontally aligned growth with size engineered catalystic nanoparticles to diameter specified growth of SWNTs

**Jin-Ju Kim**, *Kangwon National University* | **Goo-Hwan Jeong**, *Kangwon National University*

Single-walled carbon nanotubes (SWNTs) have been widely studied due to their outstanding properties and potential applications in many areas. Since their electronic, physical and optical properties are decided by their diameter and chirality, a number of researches to control the diameter or chirality has been dedicated so far. More specifically, owing to their correlation between tube diameter and catalyst size, a lot of experimental and theoretical works have focused to more clarify the size relations between them and great progress is recently undergoing. According to this background, we investigated the catalyst particle size effect on SWNT diameter systematically. We used spin-coated ferritin molecules with optimized conditions to get monodispersed catalytic nanoparticles on substrates. In addition, the size of the catalytic iron nanoparticles was controlled by high temperature annealing under argon atmosphere. The proportionality between annealing time and particle size reduction gave reliability of the treatments. Silicon with thermal oxide and ST-cut quartz wafers were used as growth substrates and their growth results such as tube diameter distribution, density and yield were compared. AFM was mainly used for diameter estimation. Especially, the horizontally aligned SWNTs on the quartz substrates were transferred onto the patterned slit substrates which make quite effective to get RBM signals of Raman spectroscopy. We believe the obtained results contribute to not only size control of nanoparticles but also diameter specified growth of SWNTs.

## Poster Board | 272

### Selective growth of (6, 5) rich single-walled carbon nanotubes with Au catalyzed diffusion plasma chemical vapor deposition

**Zohreh Ghorannevis**, *Tohoku University* | **Toshiaki Kato**, *Tohoku University* | **Toshiro Kaneko**, *Tohoku University* | **Rikizo Hatakeyama**, *Tohoku University*

Narrowly (n, m) distributed single-walled carbon nanotubes (SWNTs) were successfully synthesized with an Au catalyst by diffusion plasma chemical vapor deposition (d-PCVD). In this study we utilized fluorescence spectroscopy to analyze the abundance of different semiconducting (n, m) SWNTs. Based on the systematical comparison between the growth methods (d-PCVD and thermal CVD) and catalyst types (Au and Fe), it was found that the narrow chirality distribution can be realized only when the Au catalyst is utilized in d-PCVD. Furthermore, appropriate hydrogen concentration was also found to be the critical factor for the selective growth of (6, 5) rich SWNTs. The effects of hydrogen on the chirality distribution of SWNTs were precisely investigated through the detailed plasma analysis by optical emission spectroscopy during d-PCVD. The electrical transport properties were also studied for the Au-catalyzed d-PCVD grown SWNTs.

## Poster Board | 274

### Water-free, rapid growth of millimeter-tall single-walled carbon nanotube forests: role of water for growth lifetime and nanotube structure

**Kei Hasegawa**, *The University Of Tokyo* | **Suguru Noda**, *The University Of Tokyo; PRESTO, Japan Science and Technology Agency*

Hata, Futaba, et al. realized rapid growth of millimeter-tall single-walled carbon nanotube (SWCNT) forests in 10 min by adding water during chemical vapor deposition (CVD) [1]. By controlling carbon source at low pressures, we have found a window for such growth from C2H2/Ar without water addition [2]. This time, we studied the effects of Fe catalyst thickness, C2H2 pressure and water addition on SWCNT forest growth in detail. A gradient thickness profile of Fe was prepared on Al-Si-O layer on a substrate and CVD was carried out on it. SWCNT growth was monitored in real-time by a digital camera and grown SWCNTs were analyzed at various depths from their top to bottom by Raman spectroscopy and transmission electron microscopy. SWCNTs grew to millimeter in height in tens minutes from a simple gas of C2H2/Ar, and their diameter increased from top to bottom similarly with our previous report using C2H4/H2/H2O/Ar [3]. Addition of water extended the growth lifetime only when C2H2 pressure was high whereas water degraded G/D ratios of Raman. Water little affected the diameter increase of SWCNTs from 1.5-2.0 nm at the top to 3-4 nm at the bottom of the forests, suggesting its small influence on catalyst coarsening. The simple gas condition (i.e. C2H2/Ar with or without H2O) will enable clear discussion. [1] K. Hata, et al., Science 306 (2004) 1362-. [2] K. Hasegawa, et al., A-12 in NT09, Beijing, China, June 2009. [3] K. Hasegawa, et al., T-23 in NT08, Montpellier, France, June 2008.

## Poster Board | 276

### Morphological evolution of carbon nanotube forests during chemical vapor deposition

**Phillip Vinten**, *Institute for Microstructural Sciences, National Research Council Canada; Department of Physics, University of Ottawa* | **Jeffery Bond**, *Institute for Microstructural Sciences, National Research Council Canada; Department of Physics, University of Ottawa* | **Paul Marshall**, *Institute for Microstructural Sciences, National Research Council Canada* | **Jacques Lefebvre**, *Institute for Microstructural Sciences, National Research Council Canada* | **Paul Finnie**, *Institute for Microstructural Sciences, National Research Council Canada; Department of Physics, University of Ottawa*

In situ optical microscopy of growing carbon nanotube forests reveals that the morphology of forests changes significantly as they grow and when they terminate. Forests grow at an exponentially decreasing rate before terminating suddenly and this sudden termination is accompanied by morphological changes. Morphological changes are also observed in the steady growth phase with ex situ scanning electron microscopy revealing micrometer scale features, including a periodic growth instability. Here, the nanotube forests are synthesized via water-assisted acetylene chemical vapor deposition on silicon:silicon dioxide samples patterned with thin film alumina:cobalt catalyst islands. Based on our observations, we propose that the morphological changes and sudden termination are both related to the balance of forces within the forest as it grows. We propose that the periodically wandering nanotubes are caused by a non-uniform growth rate throughout the forest and interactions between nanotubes. We conclude that optimizing nanotube forest growth requires more than simply optimizing individual nanotube growth: it also requires optimizing the collective effects of many nanotubes.

## Poster Board | 278

### Unraveling the nucleation of SWNTs: bond switching regimes in nickel and nickel-carbon nanoclusters

**Erik Neyts**, *University Of Antwerp, Department of Chemistry* | **Yasushi Shibuta**, *The University of Tokyo, Department of Materials Engineering* | **Annemie Bogaerts**, *University Of Antwerp, Department of Chemistry*

Understanding the fundamental dynamics in carbon nanotube (CNT) catalysts is of primary importance to understand CNT nucleation. This Letter reports on calculated bond switching (BS) rates in pure and carbon containing nickel nanoclusters. The rates are analyzed in terms of their temperature dependent spatial distribution and the mobility of the cluster atoms. The BS mechanism is found to change from vibrational to diffusional at around 900 K, with a corresponding strong increase in activation energy. Furthermore, the BS activation energy is observed to decrease as the carbon content in the cluster increases, resulting in an effective liquification of the cluster.

## Poster Board | 280

### Production of spinnable carbon nanotube forests on flexible, unpolished stainless steel thin foils

**Xavier Lepro**, *The University Of Texas At Dallas* | **Marcio Lima**, *The University Of Texas At Dallas* | **Ray Baughman**, *The University Of Texas At Dallas*

We report by first time a successful growth of yarn-spinnable and sheet-drawable carbon nanotube (CNT) forests on highly flexible, inexpensive stainless steel sheets, instead of the conventionally used polished silicon wafers. The controllable growth of spinnable CNT forest is challenging since minor changes in the synthesis/substrate conditions can produce unspinnable forests instead of spinnable ones. We call the property of CNT forests to self-assemble in dry state drawability. The forests obtained on metallic substrates show similar good drawability to those grown on Si substrates (Zhang et al. Science 306, 1358, 2004). However, this new process has the additional advantage of having drawable CNT forests directly grown on flexible substrates, cheaper than conventional Si wafers, which can potentiate the technological application and mass production of the aligned CNT sheets and yarns obtained from them as structural materials, transparent electrodes, actuators and others (Zhang et al. Science 309, 1215, 2005 and Aliev et al. Science 323, 1575, 2009). Due to the flexibility of the substrate, we were able to increase the area of forests up to 16 cm width by bending the substrate to fit inside the tubular quartz CVD reactor of 7 cm in diameter. Robustness of our method is shown by the growth of these drawable CNT forests on either a single or both faces of stainless steel foils by a single thermal chemical vapor deposition at atmospheric pressure.

## Poster Board | 282

### Synthesis, formation mechanism and characterization of nitrogen-doped SWCNT films

**Toma Susi**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland* | **Giorgio Lanzani**, *Thule Institute, University of Oulu, Finland* | **Paola Ayala**, *Department of Physics, University of Vienna, Austria* | **Albert Nasibulin**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland* | **Raul Arenal**, *LEM, ONERA-CNRS, France* | **Hong Lin**, *MPQ, CNRS-U, Paris, France* | **Jerome Lagoute**, *MPQ, CNRS-U, Paris, France* | **Marina Zavodchikova**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland* | **Dongming Sun**, *Department of Quantum Engineering, Nagoya University, Japan* | **Yutaka Ohno**, *Department of Quantum Engineering, Nagoya University, Japan* | **Cyrielle Roquelet**, *LPQM, ENS Cachan CNRS, France* | **Jean-Sébastien Lauret**, *LPQM, ENS Cachan CNRS, France* | **Annick Loiseau**, *LEM, ONERA-CNRS, France* | **Kari Laasonen**, *Department of Chemistry, University of Oulu, Finland* | **Esko Kauppinen**, *NanoMaterials Group, Department of Applied Physics, Aalto University, Finland*

We present a method to synthesize nitrogen-doped SWCNTs using a gas phase coating catalyst reactor. The method allows depositing the as-grown material directly on various substrates in a simple continuous process using a resistively heated iron wire/CO/ammonia system. No solution dispersion or processing is used to preserve the intrinsic properties of the material. To study the mechanisms of doping, spin-polarized periodic density functional theory (GPAW code) was employed. The bonding and chemistry of CO, NH3 and their fragments on a Fe55 icosahedral cluster was considered. Possible dissociation paths for NH3 to atomic nitrogen and hydrogen were identified. The calculated lowest reaction barrier is comparable to an experimentally determined value (0.45 eV) obtained by FTIR and mass spectrometer measurements. The CO dissociation barrier (0.63 eV) is lower than on most of the studied Fe surfaces. Possible paths for C-C and C-N bond formation were also identified and found to be barrierless. Optical absorption and Raman spectroscopy were performed on samples synthesized with varying amounts of ammonia. The nitrogen content was examined with XPS, showing that a controllable doping level was achieved. Additionally, TEM/EELS observations were combined with STM/STS in order to locally understand the role of N atoms at the dopant sites. A well structured photoluminescence signal was observed, demonstrating that low enough doping level preserves the electronic structure of the SWCNTs. Finally, we studied the electrical properties of the films for possible application as transparent conductors and thin film transistors.

## Poster Board | 286

### Direct synthesis of single-walled carbon nanotube probes for local probe methods by Hot Filament CVD : Set up duplication

**Sophie Marsaudon**, *Université Bordeaux 1 CBMN - UMR 5248* | **Anne-Marie Bonnot**, *Université Bordeaux 1 CBMN - UMR 5248* | **Julien Buchoux**, *Université Bordeaux 1 CBMN - UMR 5248* | **Touati Douar**, *Université Bordeaux 1 CBMN - UMR 5248* | **Jean-Pierre Aimé**, *Université Bordeaux 1 CBMN - UMR 5248*

The constraints for the realization of atomic force microscopy (AFM)probes are numerous : there should be one nanotube , perpendicular to the surface, well attached to the end of a cantilever, and with a length as short as possible. Growth on AFM probes with catalytic layer has demonstrated to lead to a sufficient rate of success on a modified reactor . We are duplicating this reactor.

## Poster Board | 288

### Nanotube formation from C70 molecules in confined medium: In-situ analysis of high temperature transformation of C70 peapods

**Pascale Launois**, *Laboratoire de Physique des Solides, UMR CNRS 8502, France* | **Colin Bousige**, *Laboratoire de Physique des Solides, UMR CNRS 8502, France; ILL, Grenoble, France* | **Bart Verberck**, *Departement Fysica, Universiteit Antwerpen, Belgium* | **Dorothée Colson**, *SPEC, France* | **Julien Cambedouzou**, *Laboratoire de Physique des Solides, UMR CNRS 8502, France*

Nanotube formation in confined medium, from molecules inside single-walled carbon nanotubes, has been extensively studied experimentally and theoretically for C60 molecules but it is not yet understood for other molecules. New results concerning C70 peapods transformation into double-walled carbon nanotubes (DWCNT) are reported. Comparative X-ray diffraction (XRD) studies of DWCNT made from C60 and from C70 peapods show that their structures are the same for a given temperature of transformation [1]. The inner tube diameter is fixed by the outer tube diameter, acting as a template, and it can be tuned by changing the temperature of transformation [2]. The formation mechanism may however be specific in the case of C70 peapods due to specific molecular chemical reactivity. We present here the first in-situ XRD study of the transformation together with Monte-Carlo simulations of molecular re-orientations prior to the transformation [2]. New models developed to analyse the XRD patterns allow us to study intermediate states of the reaction and its kinetics. The amount of tubes or portions of tubes formed as a function of time, at constant temperature, is determined [2]. Based on our experimental results, possible mechanisms for C70 molecules coalescence and transformation into a nanotube are proposed, leading to a unified view of the formation of DWCNT from both C60 and C70 peapods. Opened questions concerning kinetics will be addressed to chemists and theoreticians. [1] P. Launois et al., Carbon 48, 89 (2010) [2] Articles in preparation

## Poster Board | 292

### Synthesis and characterization of TWNTs derived from thermal treatment of DWNTs-peapods

**Hiroyuki Muramatsu**, *Shinshu University* | **Takuya Hayashi**, *Shinshu University* | **Kim YoongAhm**, *Shinshu University* | **Morinobu Endo**, *Shinshu University*

Synthesis of triple walled carbon nanotubes has been considered one of the main challenges. The tri-coaxial structure is predicted to show fascinating unique physicochemical properties compared with single and double walled carbon nanotubes. In this study, we report synthesis and structural characterization of TWNTs derived from thermal treatment of DWNTs-peapods by TEM, Raman, PL, and UV.

## Poster Board | 294

### Effect of carbon black structure and impurity content on SWCNT production by RF induction thermal plasma

**Yasaman Alinejad**, *Université de Sherbrooke* | **Gervais Soucy**, *Université de Sherbrooke* | **Nathalie Faucheux**, *Université de Sherbrooke*

Due to the increasing worldwide industrial demand for Single-Walled Carbon Nanotubes (SWCNTs), it has become inevitable to develop rapid and efficient synthesis methods utilizing inexpensive starting material such as carbon black which has relatively low cost and market availability. In this work, SWCNTs have been synthesized with eight different types of carbon blacks in order to investigate effects of carbon black micro-structure and impurity content on the SWCNT formation in the RF induction thermal plasma process which is a promising technique for large scale high quality SWCNTs production. SWCNTs are produced by the direct evaporation of a mixture of carbon black and catalysts (i.e., a ternary mixture consisting of Ni, Co, and Y2O3) inside the plasma plume. The properties of the raw materials and products have been studied by the means of many characterization techniques such as, X-ray diffraction, and Raman spectroscopy. Thermodynamic equilibrium compositions of a mixture of carbon black and catalysts used as a feedstock were calculated theoretically to obtain a better understanding of the effects of carbon black grades on SWCNT production. Both experimental and theoretical results show that the physico-chemical properties of the carbon blacks such as particle size, sulphur content, and grain size, all have significant effects on the quality of the SWCNT produced. Carbon blacks with smaller particle and grain sizes, and sulfur impurity content of 1 – 2 wt%, can produce better quality SWCNTs. However, carbon black properties seem to have a negligible effect on the diameter distribution of the SWCNT.

## Poster Board | 296

### Investigation of the effect of various parameters in deposition of carbon nanotubes using dielectrophoresis

**Ali Kashefian Naieni**, *Department of Electrical and Computer Engineering, University Of British Columbia* | **Alireza Nojeh**, *Department of Electrical and Computer Engineering, University Of British Columbia*

For carbon nanotubes to be used in many electrical and optical applications, they need to be connected to a pair of electrodes. Although there have been many efforts in developing methods to make selective and reproducible deposition of nanotubes possible, a perfectly reliable method is still not available. Dielectrophoresis (DEP) can be used to apply an electric force to nanotubes suspended in a solution, and attract them towards electrodes. This technique has been used extensively to make nanotube-based devices such as field-effect transistors. Despite the important role of DEP, systematic studies on the effect of various parameters involved in it are rare. Here, we report a systematic investigation of the effects of the amplitude and frequency of the applied field, as well as the process time, in the deposition of carbon nanotubes from solutions made using two of the most popular surfactants, SDS and SDBS. To have a single nanotube bridge the two electrodes, we report a suitable range of the applied field, which depends on the frequency. For example, using the SDBS solution at 2 MHz (DEP force positive on metallic tubes but negative on semiconducting tubes), this window is between 0.8 and 1 V/um. This range is from 1.1 to 1.4 V/um at 500 KHz (DEP force positive for both type of nanotubes). Selective electrical breakdown can be used to eliminate metallic tubes in case only semiconducting ones are needed. The effect of biasing the gate to protect semiconducting tubes during electrical breakdown is also discussed.

# Friday, July 2

## 10:01-11:30 Poster Session 6

### Poster Board | 3

#### Stable, self-ballasting field emission from zinc oxide nanowires grown on an array of vertically-aligned carbon nanotubes

**Yan Zhang**, *University of Cambridge* | **Chi Li**, *University of Cambridge* | **Mark Mann**, *University of Cambridge* | **Gehan A.J. Amaratunga**, *University of Cambridge* | **William I. Milne**, *University of Cambridge*

A novel structure composed of zinc oxide nanowires (ZNWs) grown hydrothermally on an array of vertically-aligned carbon nanotubes (CNTs) was fabricated and its field emission properties determined and compared with bare CNT arrays. The combination produced a macroscopic turn-on field of 1.2 V/_m which was found to be the lowest reported from ZNWs deposited on a 2D substrate and much less than the equivalent CNT array (5.2 V/_m ). Crucially, field emission was found to be much more stable at higher pressures of 5x10^-6 mbar without exhibiting current degradation for a fixed external field, whilst emitting with a current density of 1 mA/cm2, the current density typically required for backlighting and field emission displays. We propose a self-ballasting mechanism, in which the low carrier density in the zinc oxide prevents current runaway in the presence of adsorbed species.

### Poster Board | 6

#### Characterization of length sorted DNA-wrapped single-wall carbon nanotubes for thin film transistors

**Yuki Asada**, *Department of Chemistry, Nagoya University* | **Yasumitsu Miyata**, *Department of Chemistry, Nagoya University* | **Kazunari Shiozawa**, *Department of Chemistry, Nagoya University* | **Yutaka Ohno**, *Department of Quantum Engineering Nagoya University* | **Ryo Kitaura**, *Department of Chemistry, Nagoya University* | **Toshiki Sugai**, *Toho University* | **Takashi Mizutani**, *Department of Quantum Enhineering Nagoya University* | **Hisanori Shinohara**, *Department of Chemistry, Nagoya University*

The preparation of large scale and uniform networks of single-wall carbon nanotubes (SWNTs) is very important for high performance electronics such as thin film transistors (TFTs), aimed at potentially replacing silicon devides in the future. To maximize the performance of SWNT-TFTs, it is desireble to obtain SWNTs of similar diameter and chirality for obtaining sufficient on-currents and reproducible device characteristics. The length of SWNTs should also be controllable to meet the requirement of desired channel length. We have reported that high performance SWNT-TFTs using DNA-wrapped SWNTs (DNA-SWNTs) which can provide an effective way to fabricate the uniform networks of highly isolated, structure-sorted nanotubes for TFTs. Here, we report the fabrication of SWNT-TFTs and the comparison of the transistor performance among devices of various SWNT density and length. We prepared two different DNA-SWNT lengths of 200 and 400 nm using size exclusion chromatography. DNA-SWNT networks were formed on an amino-coated SiO2 substrate, and the nanotube density was also controlled by changing deposition times. The detail results of the density and length dependence will be discussed.

### Poster Board | 9

#### Non-lithographic patterning of carbon nanotube networks via electrodynamic focusing during deposition

**Marina Zavodchikova**, *Nanomaterials Group, Department of Applied Physics and Center For New Materials, Aalto University School of Science and Technology, Finland* | **Kestutis Grigoras**, *Microfabrication Group, Department of Micro and Nanosciences, Aalto University School of Science and Technology, Finland* | **Albert G. Nasibulin**, *Nanomaterials Group, Department of Applied Physics and Center For New Materials, Aalto University School of Science and Technology, Finland* | **Ville Hurskainen**, *Nokia Research Center, Finland* | **Vladimir Ermolov**, *Nokia Research Center, Finland* | **Esko I. Kauppinen**, *Nanomaterials Group, Department of Applied Physics and Center For New Materials, Aalto University School of Science and Technology, Finland*

Carbon nanotube networks (CNTNs) have been widely studied due to their potential for low-cost applications in electronics, enabling large area coverage, structural flexibility and low-temperature processing. The successful implementation of CNTNs in devices requires the ability to pattern the networks into various features at desired locations on the substrate. Owing to the earlier demonstrated efficient and density-controlled dry deposition method of SWCNTs at room temperature directly from the aerosol synthesis reactor onto any type of substrate[1], we were able to achieve the direct CNTN patterning simultaneously with the deposition process in gas phase by means of a shadow mask and fabricate CNTN-based transistors eliminating photolithography or etching processes. The patterning method is based on electrodynamic focusing concept for charged aerosols[2]. Due to the spontaneous charging phenomenon of SWCNT bundles[3], charge is accumulated on the mask surface during the CNT deposition, modifying the applied electric field to produce electrostatic lenses around the mask opening. Thus CNTs are efficiently focused into the mask opening and onto the collecting substrate, producing feature sizes of the obtained patterns smaller than the ones on the mask. The experimental results were verified by numerical simulations of electric field distribution. Therefore, by controlling the electric field-induced motion of CNTs, we can selectively deposit CNTNs and scale down the features of CNT patterns, overcoming the mask resolution limits, which is advantageous for various electronic applications. [1] M.Y.Zavodchikova et al, Nanotechnology 20, 2009 [2] H.Kim et al, Nature Nanotechnology 1, 2006 [3] A.G.Nasibulin et al, J.Phys. Chem.C 112, 2008

### Poster Board | 12

#### Controlled growth of semiconducting single-walled carbon nanotubes by diffusion plasma chemical vapor deposition

**Makoto Akutsu**, *Department of Electronic Engineering, Tohoku University, Japan* | **Toshiaki Kato**, *Department of Electronic Engineering, Tohoku University, Japan* | **Syunsuke Kuroda**, *Department of Electronic Engineering, Tohoku University, Japan* | **Toshiro Kaneko**, *Department of Electronic Engineering, Tohoku University, Japan* | **Rikizo Hatakeyama**, *Department of Electronic Engineering, Tohoku University, Japan*

Since single-walled carbon nanotubes (SWNTs) have great and unique electrical properties, high performance SWNTs field effect transistors (SWNTs-FETs) are expected to be developed as a critical component of next-generation nano electronics. On purpose to realize the high performance SWNTs-FET, it is necessary to selectively utilize semiconducting SWNTs as a channel of FET. Although several groups reported the preferential growth of semiconducting SWNTs by plasma chemical vapor deposition (CVD), the detailed mechanism for this phenomenon still remains to be clarified. Based on this background, we investigate electrical transport properties of thin film SWNTs-FETs by aiming at the diameter distribution of SWNTs grown by diffusion plasma CVD. The SWNTs production is carried out on a Co 0.2 nm/SiO2 300 nm/Si substrate. SWNTs-FETs are fabricated by forming source and drain electrodes (Pd) on the top of SWNTs films using photo-lithography. The SWNTs diameter tends to increase with an increase in the growth temperature. The SWNTs-FETs consist of large diameter SWNTs are found to show good performance compared with the other devices made by relatively small diameter tubes. This can be explained by the difference of the defect formation rate depending on the tube metallicities and diameters.

### Poster Board | 15

#### Tube-to-tube and metal-to-tube contact influence on the performance of carbon nanotube network transistor

**Kestutis Grigoras**, *Department of Micro and Nanosciences, Aalto University School of Science and Technology, Espoo, Finland* | **Marina Zavodchikova**, *Laboratory of Physics and Center for New*

*Materials, Aalto University School of Science and Technology, Finland* | **Esko Kauppinen**, *Laboratory of Physics and Center for New Materials, Aalto University School of Science and Technology, Finland* | **Vladimir Ermolov**, *Nokia Research Center,Finland*

Thin film transistor (TFT) is one of the most attractive and widely exploited applications of single-walled carbon nanotube networks (SWNTNs). Different types of substrate, different nanotube growth techniques as well as different ways to form the transistor's channel result in different performance of the device. The understanding of operation principles and electrical transport of the channel formed by nanotubes is important achieving desired functionality and further improvements. In the case of just a single nanotube transistor the switching mechanism is dominated by the modulation of the Schottky barriers formed at the metal-nanotube interface. However, the electrical transport in SWNTN based transistor is more challenging due to the presence of multiple tube-to-tube contacts, with Schottky barriers formed at the junctions of semiconducting and metallic tubes as well as at the interface of the metal contacts. In this work we investigate the operation mechanism of SWNTN TFT in more details. The transistor channel was obtained by direct dry deposition of SWNTs using aerosol method [1]. The main aim is to distinguish between influences of two channel areas on the transistor's performance: the interface to electrode area (metal-to-tube contacts) and the central area (tube-to-tube contacts). This is achieved by designing different gate shapes which affect only the selected area of the channel. Thus we are able to selectively modulate the Schottky barriers formed at metal-to-tube or tube-to-tube contacts in order to determine their role in the switching mechanism of SWCNTN TFTs. 1. M Y Zavodchikova et al, Nanotechnology 20, (2009), 085201

## Poster Board | 18

### Carbon nanotube field effect transistor and microelectromechanical system based non-volatile memory

**SeungJoo Park**, *Seoul National University* | **Sang Wook Lee**, *Konkuk University* | **Eleanor E. B. Campbell**, *Konkuk University; University of Edinburgh* | **Yung Woo Park**, *Seoul National University*

A new nonvolatile memory device made of microelectromechanical (MEM) system and carbon nanotube (CNT) field effect transistor (FET) is developed. The control gate in conventional flash memory device is replaced with a MEM cantilever. CNT is used as the active channel between the source and drain, and Au floating gate is controlled by the MEM cantilever. The MEM cantilever is pulled down by external field applied from the bottom electrode. The set and reset current can be stored in the Au floating gate. In this presentation, the several nonvolatile memory properties of our CNT-FET based MEM device such as writing/erasing opertaion, persistent time, operating speed, and multinary bit operation are discussed.

## Poster Board | 21

### Preparation of transparent SWCNT electrode for tactile touch screen

**Kunnyun Kim**, *Korea Electronics Technology Institute* | **Kwonwoo Shin**, *Korea Electronics Technology Institute* | **Song Yi Han**, *Korea Electronics Technology Institute* | **Jong Hun Han**, *Korea Electronics Technology Institute*

Single walled carbon nanotube (SWCNT) transparent electrode was prepared for tactile touch screen which is touch screen input device and is also detectable of touch pressure. Tactile touch screen was composed of deformable upper SWCNT electrode, lower ITO electrode, and compressive-elastic layer between electrodes. In order to prepare SWCNT upper electrode, thermally purified arc-SWCNT was dispersed in water using surfactant and deposited on PET substrate by spraying coating method. The resulting SWCNT layer showed the sheet resistance of 590 Ohm/sq and the light transmittance of 86.1% measured at 550nm wavelength. SWCNT electrodes were patterned by laser scribing method. SWCNT electrodes on PET were deformed by external touch force, which resulted in the capacitance change by changing gap between upper and lower electrodes. In order to obtain the higher sensitivity, we selected compressive-elastic gel with the high rate of the capacitance change. In result, we could obtain the capacitance variation from 1.92pF to 3.42pF when the applied force varied from 0 to 5N.

## Poster Board | 24

### Electronic properties control of single-walled carbon nanotube using spontaneous redox process of MnO4- and carbon nanotube

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Single-walled carbon nanotube (SWCNT) thin film is three dimensional interconnected networks of quantum wires and a large number of factors can affect their optical and electrical properties. In order to obtain the low sheet resistance of SWCNT thin film that has the high transmittance at 550 nm, electronic properties of SWCNTs film are modified through chemical treatment and enhanced carrier injection. We investigated the effectiveness of electronic properties with single-walled carbon nanotube through spontaneous redox reaction between the metal oxide ion such as MnO4- and carbon nanotube. The SWCNTs synthesized by the arc discharge method were used. The SWCNT powder was dispersed with sodium dodecylbenzene sulfonate (SDBS) in deionized water and sonicated, followed by the centrifugation. The SWCNTs film has been fabricated by a filtration-wet transfer method on a various substrates such as glass, Si wafer, and polyethylene terephthalate (PET). The sheet resistance of SWCNTs film decorated with MnO2 has lower than that of as-prepared SWCNTs film. The effect of doping on electronic structure of SWCNTs was investigated by four point probe (FPP), UV-vis-NIR absorption spectrometer, and Raman spectroscopy and SWCNTs film decorated with MnO2 was characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

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### High current field emission of filtrated carbon nanotube emitters supported by a metal mesh

**Hansung Lee**, *Sejong University* | **Jeungchoon Goak**, *Sejong University* | **Jusung Choi**, *Sejong University* | **Chungyeol Lee**, *Sejong University* | **Naesung Lee**, *Sejong University*

Carbon nanotubes (CNTs) have been studied long to be applied as field emitters for backlight units (BLUs), lighting lamps, X-ray sources, microwave amplifiers, electron microscopes, etc. The X-ray tubes have been attempted to be fabricated by using a CNT emitters for micro-focusing and power saving. Recently, CNT emitters looked toward producing high emission currents to provide X-ray dose enough for specific applications. However, many researchers reported the degradation and failure of CNT emitters during extraction of high current emission. We have tried to fabricate X-ray source CNT emitters with high current emission and long-term stability. In this study, a CNT emitter was fabricated by filtrated stable CNT solution with a metal mesh and then fixed on a metal substrate for micro-patterning and enhancing adhesion. The stable CNT solution was made by ultrasonic dispersion and centrifugation. The CNT emitters were activated with an adhesive tape, following the firing at 450°C. The field emission was measured in a diode configuration by applying dc voltages in a vacuum chamber with a pressure level of ~10-7 torr. The effect of added to stainless steel would also be discussed in detail in comparison to conventional filtrated CNT emitter.

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### Composite Reduced Graphene Oxide and Nanotube Transparent Electrodes for use in Flexible Organic Electronic Devices

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Graphene, a monatomic layer of carbon atoms, has become one of the most promising materials in nanotechnology due to its superb mechanical and electrical properties. There are various graphene fabrication techniques including mechanical and chemical exfoliation of graphite as well as chemical vapour deposition (CVD). Mechanical exfoliation yields the highest purity graphene but yields small area flakes of graphene. CVD yields high purity, large area graphene films however transfer methods are currently complicated and impractical and CVD is a high temperature, low pressure process. Chemical exfoliation is a relatively low purity process yet results in large area films at STP. Furthermore, a chemical processes is easily scalable for purposes of mass production. For these reasons, we employ a chemical exfoliation process to fabricate graphene (by means of reduced graphene oxide (RGO)) for use as the transparent electrode in organic electronic devices such as solar cells and organic light emitting diodes (OLEDs). To combat the poor electronic properties of RGO, we combine RGO with single-walled carbon nanotubes (SWNTs) in an effort to short-circuit flakes of graphene together thus improving the sheet resistance over the entire film. We compare the sheet resistance, optical transparency, and thickness between RGO films, single walled carbon nanotubes (SWNTs) films, and two different composite RGO-SWNT structures and show the ameliorated effects of our composite structure. Due to the low temperature fabrication process we are able to transfer these electrodes to flexible substrates (such as PET) and compare the performance of each electrode in organic devices.

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### Interface charges as a key factor to realize high-performance carbon nanotube FETs for CMOS applications

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We have realized high-performance p-type and n-type top-gate CNFETs with an $Al_2O_3$ and $HfO_2$ gate insulators, respectively. CMOS inverters with a high gain and a large noise margin have also been fabricated by integrating $HfO_2$-gate and $Al_2O_3$-gate CNFETs on a single SWNT. It is shown that the carrier type of CNFETs depends on fixed charge density at the interface between the gate insulator and a $SiO_2$ layer of a Si substrate. This technique to control the carrier type is stable in air and compatible with Si CMOS process technology. We also suggest that in the presence of interface fixed charges, the operation mechanism of CNFETs changes from the Schottky barrier modulation to the channel modulation, and the ambipolar conduction can be suppressed due to the high-potential region formed near the contact electrode.

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### Field-effect-transistor controlled field emission from SWCNTs

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A new emission current control technique with embedded FET structure is proposed for field emission devices based on 1D nanomaterials such as carbon nanotubes (NT). The body of the NT serves as the channel of the FET with gate structure and the tip as the field emitter. For any given field emission action, the NT tip potential maintains a self-consistent equilibrium condition and the emission current is exclusively supplied by the current flowing through the NT-FET channel. The discrete density-of-states of the 1D semiconducting NT allows the FET to operate in the quantum capacitance limit that facilitates effective band engineering inside the channel. The gate bias modulates the contact or transport characteristics of the NT-FET and hence manages the current supply to the field emitter tip. Depending on the contact material, gate structure and bias conditions, the NT FET operates as a conventional FET or Schottky barrier FET and can be subject to different transport modes such as ballistic transport, multiband transport, band-to-band tunneling and avalanche impact ionization, and the current vs. gate voltage characteristics of the FET would present in the overall field emission device performance. This is estimated by the simulations and demonstrated by the experimental results. Such design provides a simple device structure offering high-sensitivity and well-defined field emission current control from NTs, which is desirable for many field emission applications.

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### Mechanical, electronic and transport properties of carbon nanotubes in a cross structure

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Due to their quasi one-dimensional nature, nanotubes are ideal candidates for making quantum devices. A nanotube cross is a structure made by a carbon nanotube passing over another one at an angle. Because of the induced mechanical deformation at the intersection point, the electronic properties of the nanotubes in a cross could vary significantly from those of intact nanotubes, potentially leading to the formation of nanoscale quantum dots. We report a theoretical study of the mechanical, electronic and transport properties of semiconducting and metallic nanotubes in a cross structure. Physically viable and stable configurations were found using molecular dynamics simulations. It was observed that the final configuration the nanotube relaxes to does not depend strongly on the initial guess for its shape. The electronic structure of the most deformed part of the top nanotube in the cross was then found using first-principles calculations. Band gap change as a result of deformation was observed in tubes with various chiralities and different degrees of deformation. The current-voltage characteristics of the deformed nanotubes were then calculated using a transport solver developed in-house. This code uses the results of the first-principles simulations of the electronic structure in a nonequilibrium Green's function formalism with a three–dimensional, real-space basis. The transmission probability of electrons through the deformed nanotubes as a function of applied voltage is calculated and the total current obtained through the Landauer-Buttiker formula. The changes in the transport characteristics of different carbon nanotubes with various levels of deformations are discussed.

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### Multiwall carbon nanotubes photocathodes : Modulation of multiwall carbon nanotubes field emitted electron beam using laser illumination

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MWCNTs are excellent field emitters. They are whisker-like in shape with very high aspect ratio, leading to high field enhancement at their apexes. They are arguably the most stable and robust cold field emitters known. A maximum emission current of 100–200 µA per individual MWCNT and current density of 1A/cm² in DC mode for MWCNTs array have been demonstrated. However, many applications require high frequencies modulation of the electron beam. In 2007, Nanocarb, a Thales R&T-LPICM joint laboratory, demonstrated using a resonant cavity the modulation at 32GHZ of a 1.4A/cm2 peak current density with a 82% modulation ratio. For large bandwidth microwave amplifiers, resonant devices can not be used. In order to extend the application domain, Nanocarb proposes to use optically driven cathodes. This novel photocathode concept which consists in a MWCNT array, where each MWCNT is associated with one p–i–n photodiode. The photon–electron conversion is achieved using the p–i–n photodiodes whereas the electron emission occurs from the MWCNTs. To demonstrate this new photocathode concept, Nanocarb fabricated the first CNT photocathode using silicon p-i-n photodiodes. Using a red laser, this photocathode delivers 0.8mA with a ION / IOFF ratio of 25 and exhibit an internal quantum efficiency of 10%. By incorporating high frequency p–i–n photodiodes (e.g. GaInAs photodiodes) into the structure and driving them with 1.55 µm telecommunication lasers, photocathodes operating in the 10-40 GHz frequency range can be expected.

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### Carbon nanotube-counter electrodes of dye-sensitized solar cell

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Since first discovery of carbon nanotubes(CNTs) by ijima[1], CNTs have fascinating many researchers because of their excellent properties such as mechanical strength, thermal stability, and electrical conductivity. Especially, their chemical stability, high surface area, and catalytic activity for the reduction of triiodide in redox active electrolyte[2] make them an alternative candidate for counter electrodes of dye-sensitized solar cell(DSSC). In this study, we fabricated CNT-counter electrode of DSSC by air brush method and direct growth of CNT film on FTO using CVD and investigated the energy conversion efficiency of DSSC consist of conventional TiO2 anode and CNT films on FTO glass with different thickness as counter electrodes. CNT- counter electrodes were characterized by scanning electron microscopy (SEM) and spectrophotometer. Finally, the change of catalytic activity which result from ozone or acid treatment of CNT film was studied by Raman spectroscopy. [1] S. Iijima, Nature, 354, 56-58 (1991) [2] J. E. trancik et al. Nano Lett., 8, 982-987 (2008)

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### Dissolution of Relatively Long Single-walled Carbon Nanotubes and Application to Transparent Electrodes

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Successful fabrication of CNT electrodes with low surface resistance and high visible-light transmission depends critically on making good CNT dispersion solutions without cutting CNTs too short via excessive ultrasonication. Therefore, it is highly preferable to employ the technique with low power and short-term ultrasonication. In this study, CNT was dispersed in 1,2-dichloroethane by adding poly(m-phenylenevinylene-co-2,5-dioctyloxy-p-phenylene vinylene) (PmPv) as a dispersing agent via ultrasonic agitation within 1.5 hours. It resulted in high density of individual CNT with mean length of about 3.5 microns. Our SWCNT films fabricated by spincoating using this solution showed visible-range transmittance of about 85% at sheet resistance of about 80 ohm/sq. Furthermore, we will discuss the performance of OLEDs and Organic solar cell based on as-prepared CNT transparent electrodes.

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### Fabrication of Highly Conductive and Transparent Carbon Nanotube Thin Films using Layer-by-Layer Self Assembly Method

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Transparent conducting thin film (TCF) has wide applications in transparent conducting electrode, touch screen, electromagnetic wave shielding film, photovoltaic cells and polymer light emitting diodes. The most widely used material for TCF are metal oxides which have strong disadvantages due to their limited quantity and difficulty to fabricate large area films. Carbon nanotubes (CNT) are another strong candidate for alternative material due to their outstanding electrical and optical properties and high aspect-ratio. Fabrication of TCF using CNT has been tried using vacuum filtration, transfer printing, spin-coating, and drop casting. However, these fabrication techniques have not provided the full requirements for a transparent conducting electrode yet. In this study, single-wall carbon nanotubes (SWNT)/polyelectrolyte multilayer films with good electrical and optical properties were successfully fabricated using the layer-by-layer self-assembly method. The fabrication method and the electrical and optical properties of fabricated thin films will be presented.

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### Ultrafast energy transfer at a single-walled carbon nanotube-polymer molecular junction

**Samuel Stranks**, *University Of Oxford* | **Christian Weisspfennig**, *University Of Oxford* | **Patrick Parkinson**, *University Of Oxford* | **Michael Johnston**, *University Of Oxford* | **Laura Herz**, *University Of Oxford* | **Robin Nicholas**, *University Of Oxford*

We report an ultrafast energy transfer process between a single-walled carbon nanotube (SWNT) and a dispersing semi-conducting polymer, poly(3-hexylthiophene) (P3HT), three orders-of-magnitude faster than reported previously for other SWNT-polymer systems. This composite is a promising candidate for use in organic photovoltaics (OPVs). However, despite reports that there can be a type-II heterojunction alignment between the two materials, OPV devices to date have shown poor performances. In this work, we study purified P3HT-SWNT nanohybrid structures. We use photoluminescence measurements to observe the quenched polymer emission and subsequent nanotube emission following energy transfer. Femtosecond up-conversion spectroscropy is used to monitor the quenched time-decay of the polymer emission and transient absorption studies are used to probe for charge on the P3HT resulting from charge separation processes. The photoluminescence measurements show that efficient energy transfer occurs from excitation of the wrapping P3HT polymer to the SWNTs and this transfer occurs on a 430 fs time scale. The transient absorption studies demonstrate a significant initial charge generation but that this decays away rapidly. We conclude that the energy transfer process occurring between the P3HT polymer and SWNT dominates over the short-lived charge transfer and this explains the poor OPV efficiencies observed to date. The energy transfer is an ultrafast process due to intimate wrapping of the polymer around the SWNT leading to Förster-type resonant energy transfer. Our results show that the development of SWNT-based OPVs require use of smaller-diameter tubes, alternative polymers, or an altered geometry, all with the aim to facilitate longer-lived charge separation.

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### Infrared sensors based on single wall carbon nanotube films

**Charlie Koechlin**, *Onera, chemin de la hunière, France* | **Sylvain Maine**, *LPN-CNRS, route de nozay, France* | **Stéphanie Rennesson**, *Onera, chemin de la hunière, France* | **Riad Haidar**, *Onera, chemin de la hunière, France* | **Brigitte Trétout**, *Onera, chemin de la hunière, France* | **Annick Loiseau**, *LEM, ONERA-CNRS, France* | **Jean-Luc Pelouard**, *LPN-CNRS, route de nozay, France*

The use of uncooled (i.e. low cost) detectors for infrared imaging (3-12 microns) has been the subject of research and development for many decades. Among them the resistive bolometer (basically, a photoresistor) is spreading in commercial applications such as driving assistance or aircraft aid, fire-fighting, night vision... These light sensors are however still plunged by their relatively low performances (sensitivity, spectral range, response time), and there is a need for new materials and/or architectures to increase their potential, while maintaining their low cost. In this context, CNT-film based devices appear as a promising solution, since they exhibit a wide-range absorption in the infrared (from 3 microns to 300 microns, due to the excitation of free carriers), a strong bolometric behavior (that we identified as a fluctuation induced tunneling through the inter-tube junctions) and good thermo-mechanical properties. Besides the influence of the CNT type (semiconductor and metallic) has been investigated on both absorption and bolometric behaviors. We thus developed the technological building blocks (film deposition and etching, electrical contacting on micrometer-scale suspended CNT ribbons) for the realization of large, uniform, and reproducible matrix of SWCNT-film infrared-bolometers. We obtain state-of-the-art results for electrical characteristics1 (specific contact resistance and resistivity dispersion), and demonstrate the first photoresponse to mid IR radiations2. Electrical and optical characteristics of matrix of bolometers based on suspended CNT films will be discussed. 1 C. Koechlin, et al., APL 96, 10 (2010) 2 S. Maine, C. Koechlin, et al., PSSC (to be published)

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### Exciton Antennae and Concentrators from Core-Shell and Corrugated Carbon Nanotube Filaments of Homogeneous Composition

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There has been renewed interest in solar concentrators and optical antennae for improvements in photovoltaic energy harvesting and new opto-electronic devices. In this work, we dielectrophoretically assemble single-walled carbon nanotubes (SWNTs) of homogeneous composition into aligned filaments that can exchange excitation energy, concentrating and funneling it to the center of core-shell structures with radial gradients in the optical bandgap. We find in such structures an unusually sharp, reversible decay in photoemission that occurs as such filaments are cycled from ambient to only 353 K, attributed to a strongly activated Auger-like component of a dual, non-radiative pathway in the filament. We show that such filaments tend to form density oscillations of 1 to 3 um spacing along their length that create spatial periodicity in the emission wavelength. Core-shell structures consisting of annular shells of (6,5) (Eg = 1.20 eV ) and (7,6) (Eg = 1.09 eV) and cores with bandgaps smaller than those of the shell (Eg = 1.02 eV (11,3) to 0.98 eV (8,7)) demonstrate the concentration concept: broad band absorption in the ultraviolet (UV)-near-infrared (nIR) wavelength regime with singular photoemission at the (8,7) SWNT (Eg = 0.98 eV). This approach demonstrates the potential of specifically designed collections of nanotubes to manipulate and concentrate excitons in unique ways.

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### Exciton-Plasmon Coupling and biexcitonic nonlinearrities in individual carbon nanotubes

**Igor Bondarev**, *North Carolina Central University* | **Lilia Woods**, *University of South Florida* | **Kevin Tatur**, *University of South Florida*

We study theoretically the interactions of excitonic states with surface electromagnetic modes of small-diameter (~1nm) semiconducting single-walled carbon nanotubes (CNs). We show that these interactions can result in strong exciton-interband-surface-plasmon coupling in individual CNs[1]. The quantum confined Stark effect with an electrostatic field applied perpendicular to the CN axis can control the exciton-plasmon coupling strength, and exciton emission accordingly[2]. We further extend our studies to analyze the interactions of biexcitons (observed recently in single-walled CNs by the femtosecond transient absorption spectroscopy technique[3]) with the interband-surface-plasmon modes. We show the biexciton-plasmon coupling tunability by means of the quantum confined Stark effect, both for the ground-ground state and for the ground-excited state biexcitonic configurations. We expect our results to open up paths to new tunable optoelectronic device applications of small-diameter semiconducting CNs, including the strong-excitation regime with optical non-linearities. Supported by NSF (HRD-0833184), NASA (NNX09AV07A), and ARO (57969-PH-H). [1] I.V.Bondarev, K.Tatur, and L.M.Woods, Optics Commun. 282,661 (2009). [2]I.V.Bondarev, L.M.Woods, and K.Tatur, Phys. Rev. B 80,085407(2009). [3]D.J.Styers-Barnett, S.Pellison, B.P.Mehl, et al., J.Phys. Chem. C 112,4507(2008).

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### Intrinsic and Extrinsic Factors which Affects the Optical Properties of Individual Single-Walled Carbon Nanotubes

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Multiple studies have shown that the optical properties of single-walled carbon nanotubes (SWNTs) are excitonic in nature. However, a complete understanding of how these excitonic states shape the optical properties of SWNTs is lacking. Comparing the results of different published studies is difficult; the luminescence properties of SWNTs are affected by various extrinsic factors originating from synthesis and processing methods which affect the structure, sidewall quality, and environment of SWNTs. Here we use single molecule imaging and time resolved spectroscopy, photoluminescence maps, UV-vis absorbance, and Raman spectroscopy at multiple excitation wavelengths to identify different extrinsic factors which deeply influence the optical properties of SWNT. Single molecular studies of individual (6,5) SWNTs showed that SWNT luminescence depends strongly on extrinsic and intrinsic factors such as sample preparation, sample environment, sidewall defects, and tube synthesis methods (HiPco or CoMoCat). Ensemble measurements showed compelling spectroscopic evidence of substantial differences in chirality and diameter distribution which alter the luminescence properties within different

HiPco batches. These variations also affect SWNT solubility both in surfactant suspensions and superacids.

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### Auger-Ionization and Photocurrents in Single-Walled Carbon Nanotubes

**Satoru Konabe**, *Tokyo University Of Science* | **Takahiro Yamamoto**, *The University of Tokyo* | **Kazuyuki Watanabe**, *Tokyo University Of Science*

The optical properties of carbon nanotubes (CNTs) have been attracting a great deal of attention as next generation optoelectronic devices. Because of a strong coulomb interaction originating from the quasi-one-dimensional structure of CNTs, the dominant excitation by the photo irradiation is not a single-particle excitation but the elementary excitation referred to as an exciton. For an application to the photo-detector, however, the excitons do not contribute to the photocurrent unless it is dissociated into an unbounded e-h pairs, which are freely accelerated by the external electric field. In the present paper, we focus on a novel carrier-generation mechanism, the highly efficient Auger ionization process, based on the intrinsic properties of CNTs, due to the strong exciton-exciton interaction [1]. We first show the importance of the Auger ionization process in CNTs by the tight-binding calculation [2]. We then calculate photocurrents in CNTs by solving the rate equations combined with the Bethe-Salpeter equation taking account of exciton dissociation by the Auger ionization processes. We found that (1) the exciton-dissociated photocurrent abruptly increases at the threshold intensity of irradiation laser, and (2) beyond the threshold intensity, the photocurrents of excitons are around one order larger than those of the e-h pair. This indicates that the strong Coulomb interaction makes it possible to use the excitonic state as an abundant supply of carriers. [1] S. Konabe, T. Yamamoto, and K. Watanabe: Appl. Phys. Express 2, 092202 (2009). [2] S. Konabe, T. Yamamoto, and K. Watanabe: Jpn. J. Appl. Phys. 49, 02BD06 (2010).

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### Nonradiative exciton decay dynamics in single-walled carbon nanotubes

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We studied nonradiative exciton dynamics in single-walled carbon nanotubes (SWNTs) due to hole-doping [1] and exciton diffusion to ends of SWNT [2], respectively. The intensities of photoluminescence (PL) peaks decreased and the PL lifetimes became shorter with an addition of hole dopant tetrafluorotetracyano-p-quinodimethane (F4TCNQ). We found that the nonradiative decay of excitons induced by the F4TCNQ was of the order of a few tens of picoseconds for densities of ~0.1 hole/nm at room temperature, which could be explained by phonon-assisted indirect exciton ionization processes [3]. We also studied the length-dependent exciton dynamics in SWNTs using length-controlled SWNTs. From the length-dependent PL lifetimes and relative intensities, the exciton diffusion length was found to be ~50 nm, and the diffusion coefficient was ~1 cm^2/s in DNA-wrapped SWNTs. We found that the effective PL lifetimes have substantial upper limits in longer SWNTs. Our results suggest that the exciton diffusion to the ends has only a limited contribution to the net nonradiative relaxation rate, while the processes mediated by doped carriers could be a dominant origin of the efficient nonradiative relaxation in SWNTs. [1] K. Matsuda, Y. Miyauchi, T. Sakashita, and Y. Kanemitsu, Phys. Rev. B 81, 033409 (2010). [2] Y. Miyauchi, K. Matsuda, Y. Yamamoto, N. Nakashima, and Y. Kanemitsu, submitted. [3] V. Perebeinos and P. Avouris, Phys. Rev. Lett. 101, 057401 (2008).

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### Possible Observation of Inter-Shell Coupling States in Double-Walled Carbon Nanotubes

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Using a broad range of excitation wavelengths (440-850 nm), we have examined resonant Raman scattering intensities of the radial breathing modes of aqueous surfactant suspensions of double-walled carbon nanotubes (DWNTs) synthesized by chemical vapor deposition (CVD) and thermal "peapod"-coalescence techniques. Examination of the Raman excitation profiles (REPs) of specific semiconducting inner nanotubes such as the (10,2) not only reveals the observation of the expected, well-defined resonance with the second semiconducting optical transition but also the appearance of a peak at energies below the aforementioned transition but that coincide with the optical transitions of metallic outer nanotubes. This simultaneous resonance with both inner and outer walls may be evidence of electronic and/or mechanical coupling between shells. To investigate this connection further, we measured REPs of individual DWNTs deposited on a substrate using a confocal Raman microscopy with a Ti:Sapphire excitation source. The results of such measurements and their relation to the ensemble sample data will be discussed.

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### What did we learn from combined Raman and electron diffraction experiments on individual freestanding SWNTs

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We review the main information that we have obtained from Raman spectroscopy experiments combined with electron diffraction experiments on individual freestanding single-walled carbon nanotubes. This information concerns: the radial breathing mode vs diameter relationship; the dependence of the frequency and lineshape of the G-modes in semi conducting and metallic tubes; the evaluation of the optical transition energies for individual freestanding SWNTs. These experimental Raman results obtained on index-identified individual SWNTs are compared with other experimental data and theoretical predictions. The intrinsic lineshape of G-modes of the achiral and chiral, semiconducting and metallic SWNTs are unambiguously established. The results support the fact that non adiabatic effect should be taken into account to describe the diameter dependence of the LO modes of metallic SWNTs. From these data, we can also define Raman criteria that allow identifying carbon nanotubes from their Raman features only. We show the efficiency of this approach: (i) to assign the (n,m) indices of individual freestanding single-walled carbon nanotubes, and (ii) to identify the (n,m) tubes organized in a small bundle.

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### Third-Order Coherent Optical Imaging of Individual Carbon Nanotubes

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Single walled carbon nanotubes (SWCNTs) are low dimensional conductors with unique electronic and electro-optic properties. To probe these properties, we investigate the third-order, coherent anti-stokes (CAS) response of individual SWCNTs using a dual color, four-wave-mixing technique. Despite SWCNTs being nanoscale objects much smaller than the wavelength of light, the CAS response allows single SWCNTs to be optically imaged with good spatial resolution [1]. The absence of a pronounced Raman signature shows that the CAS response is dominated by electronic, rather than vibrational, dynamics. Indeed, the CAS signal allows for straightforward optical discrimination between metallic and semiconducting SWCNTs. However, variability exists in the CAS intensity that may depend on electrical contact resistances, charge carrier densities, and local physiochemical effects. Moreover, identification of the third-order CAS response in SWCNTs requires proper accounting of other non-linear processes including two-photon fluorescence.  [1] H. Kim et al, Nano Lett. 9 2991-2995 (2009)

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### Exciton effects on Raman and photoluminescence of single wall carbon nanotubes

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Resonance Raman spectroscopy and photoluminescence have been used for optical characterization and investigation of excitonic properties of single wall carbon nanotubes (SWNTs). Experiments and theories have been demonstrated a diameter and chirality dependence for resonance Raman and photoluminescence intensity of SWNTs. Excitonic effects change the intensity and optical transition energy of the photoluminescence and resonance Raman peaks. To investigate excitonic effects in resonance Raman and photoluminescence, we need to consider and calculate the intensity in the exciton picture. In this study we discuss the excitonic effects of the photoluminescence and resonance Raman intensity, and the dependence of the photoluminescence and resonance Raman intensity on diameter and chirality. Here we use the exciton-phonon and exciton-photon matrix elements in the framework of the tight-binding scheme in order to calculate the resonance Raman and photoluminescence intensity in the exciton picture. The exciton energy and exciton wave function coefficient of SWNTs are calculated by solving the Bethe-Salpeter equation in which the one particle energies are given by the tight-binding method. The screening from environment and nanotubes itself is expressed by a dielectric constant. In the calculation we change a dielectric constant to consider environmental effects. The behavior of the calculated intensity in the exciton picture reproduces the experimental results.

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### Evidence for excitons in metallic carbon nanotubes by temperature dependent Raman scattering

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Single-walled carbon nanotubes (SWCNTs) are promising candidates for a variety of applications [1]. Optical transitions play a central role in understanding the fundamental properties of carbon nanotubes and for optoelectronic devices. Both theoretical and experimental studies revealed that light absorption excites strongly correlated electron-hole pairs in semiconducting nanotubes, known as excitons, with binding energies of several hundred meV [2-5]. We present resonant Raman measurements of the optical transition energy Eii in metallic and semiconducting nanotubes at different temperatures. In semiconducting nanotubes, the transition energy decreases at high temperatures, as observed many semiconducting systems. In metallic nanotubes, on the other hand, Eii first decreases and then increases again. We interpret this unusual behavior of metallic nanotubes in terms of excitons in metallic nanotubes. We suggest that the excitons in metallic nanotubes, due to their small binding energy, dissociate into free electron-hole pairs at temperatures related to the exciton binding energy. Our results are in good agreement with theoretical predictions and experimental absorption measurements [6].   [1] S. Reich, C. Thomsen and J. Maultzsch, Carbon Nanotubes: Basic Concepts and Physical Properties (Wiley-VCH, Berlin, 2004) [2] Maultzsch et al. PRB 72, 241402 (2005) [3] Wang et al. Science 208, 838 (2005) [4] Spataru et al. PRL 92, 077402 (2004) [5] Deslippe et al. Nano Letters 8, 1626 (2007) [6] Wang et al. PRL 99, 227401 (2007)

## Poster Board | 125

### Raman intensities of the radial-breathing mode in carbon nanotubes: (n,m) abundances versus scattering efficiencies

**Hagen Telg**, *Technische Universität Berlin* | **Christian Thomsen**, *Technische Universität Berlin* | **Janina Maultzsch**, *Technische Universität Berlin*

Nanotube ensembles show strong variations in Raman intensities of the different tubes (n,m) which can either be interpreted as variations in the (n,m) abundances or variations in the scattering efficiencies. In order to address this issue we collected Raman intensities of the radial breathing mode from a large number of different tubes (n,m) (HiPCO). To collect Raman intensities from resonantly excited tubes we varied the excitation energy between 1.15 and 2.15 eV. We observe systematic variations of the Raman intensities for different (n,m) including dependences on the optical transition, diameter, family and chiral angle. Here we focus on intensity variations depending on family and  and chiral angle which we contribute to variations in the exciton-phonon coupling. In particular, we observe an intensity minimum for nantubes with chiral angle = 20o . This finding corresponds to a minimum in the exciton-phonon coupling along the K-K direction in the Brillouin zone of graphene. Furthermore we discuss intensity variations which are due to different natural electronic line widths. The line width shows a dependence on diameter and varies between metallic and semiconducting tubes.

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### Screening due to inter-wall interaction and exciton properties in double-walled carbon nanotubes

**Yuh Tomio**, *Hokkaido University* | **Hidekatsu Suzuura**, *Hokkaido University* | **Tsuneya Ando**, *Tokyo Institute of Technology*

Exciton properties in double-walled carbon nanotubes are expected to be different from those in single-walled carbon nanotubes because excitons in the inner (outer) tube are screened by electrons/holes in the outer (inner) tube through the inter-wall Coulomb interaction. In this work, we have studied effects of screening due to the inter-wall Coulomb interaction on excitons and optical spectra in semiconducting double-walled carbon nanotubes within the effective-mass theory and a static screened Hartree-Fock approximation. Our calculations clarify that the intra-wall electron-hole interaction is largely suppressed by inter-wall screening effects. The suppression is sensitive to the effective inter-wall distance between the inner and outer tubes and leads to reduce the exciton binding energy as well as the band gap energy. As a result, the exciton energy levels are redshifted slightly from those in the single-walled carbon nanotube with the same diameter. We find that the energy shift of the ground exciton has little dependence on the tube diameter, in contrast to that of the excited exciton. The exciton properties in the case of a metallic outer or inner tube, where the screening can be changed dramatically, will also be discussed.

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### Importance of Exciton Coupling on the Upper Density Limit of Optically Created Excitons in SWCNTs

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An important feature of single walled carbon nanotubes (SWCNTs) are their quasi 1-D, chiral structure which gives rise to exitonic photoluminescence from 2/3 of the species. These excitons can be created in a number of ways including electrically and optically. Future uses and technologies involving CNTs as optical emitters require an understanding of the excitonic structure and dynamics within the CNT. The excitonic structure is being extensively studied and recently an upper density limit for photo-excited excitons has been observed that is surprisingly low. This upper density limit has been explained as a diffusion limited exciton-exciton annihilation process with a diffusion length of 90 nm when observed in sodium cholate coated SWCNT in ensemble samples suspended in D2O [1]. In contrast, saturation occurs at pump fluences an order of magnitude smaller in long single air-suspended SWCNTs [(9,8), (10,8)] [2]. In Monte Carlo simulations of exciton dynamics which include dipole-dipole interactions, the excitons exhibit an attractive bias which results in an increased interaction length inversely proportional to the dielectric environment and effective mass. Experimentally the dipole interaction energy is consistent with our observation of a density dependant blue shift of emission observable only at short time delays. This is observed by a novel variant of femtosecond excitation correlation spectroscopy. [1] Murakami, Y. and Kono, J. Phys. Rev. Lett. 102, 037401 (2009) [2] Xiao, Y.-F. et al., Phys. Rev. Lett. 104, 017401 (2010).

## Poster Board | 130

### Encapsulation of Conjugated Oligomers in Single-wall Carbon Nanotubes: Toward Nanohybrids for Photonic Devices

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Building robust optoelectronic devices at the atomic scale is one of the challenges faced by nanotechnology. Single wall Building robust optoelectronic devices at the atomic scale is one of the challenges faced by nanotechnology. Single wall carbon nanotubes (SWNTs) are extremely robust nano-objects exhibiting unique electron transport, but their small band gap limits them to be near infrared emitters. In contrast, organic molecules having outstanding photophysical properties often suffer from low stability and poor electrical characteristics. Exploiting the advantages of both opens a prospective to fascinating systems with one-dimensional charge transport and light emission in the visible spectral range. A promising strategy to reach this goal is to make use of the hollow space of SWNTs to accommodate organic molecules creating a new hybrid system. We have successfully synthesized peapods combining rigid-rod like molecules such as sexithiophene with SWNTs. HRTEM and optical probes show evidence of the encapsulation, while density functional calculations confirm the experimental findings and provide deeper insight concerning stability and electronic properties of these systems. We demonstrate such nano-hybrids, emitting light in the visible range of the spectrum, as promising photon sources to be used in future opto-electronic devices.

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### Spinning CNT fiber from endlessly drawable array

**Yoku Inoue**, *Shizuoka University* | **Akihiro Ishida**, *Shizuoka University* | **Morihiro Okada**, *Shizuoka University* | **Hidenori Mimura**, *Shizuoka University*

We invented a simple one-step growth method of ultra-long vertically aligned multi-walled CNT arrays. Our method requires no pre-process for catalyst thin film (pre-deposition), and only requires iron chloride powder and acetylene gas. The MWNT array can easily be drawn into a web. The endless drawn web is easily fabricated into the nanotube fiber, tape and sheet. The MWNT array was synthesized using a thermal chemical vapor deposition system. Densely grown MWNTs are vertically aligned on a quartz substrate. The height of MWNT array reached 2.4 mm in 20 min with the high growth rate over 0.1mm/min. Drawability (spinnability) of our MWNT arrays are very high as 2 mm-long array is drawable. The CNT web is endlessly drawn by pulling out the edge of the array with no twisting. Length of the web is just limited by the amount of CNTs on the substrate. During drawing, nanotubes are drawn with taking neighbors one after another with the aid of van der Waals force. Tiny nanotubes are highly aligned in the drawing direction. Therefore large scale anisotropic CNT products are easily fabricated. The CNT fiber size is ranging from 1 to 550 tex (g/km), and the CNT sheet is as wide as A4 scale. These products are using no chemical binder. The achieved fiber strength is 340 MPa and electrical resistivity is 8.0 x 10^4 ohm•cm. Array samples are consistently drawable for each trial. Low cost, easy to scale up and highly drawable MWNT arrays promise advanced CNT products.

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### Carbon nanotube fibre: a unique high-performance yarn

**Juan Vilatela**, *University Of Cambridge* | **Alan Windle**, *University Of Cambridge*

We present results on the mechanical properties of carbon nanotube fibres produced by the Cambridge process [1]. We studied the flexibility in bending of this new material by performing knot strength tests, which consist of tying an overhand knot in fibres and comparing their tensile properties to those in the unknotted state. The results show that the CNT fibres have a high flexibility in bending, as indicated by their ability to preserve their tensile properties after being knotted. Furthermore, they indicate that the handling of this material is similar to that of conventional textile fibres (wool and cotton). These results are explained in terms of the structure of the fibres and its ability to reshape under different mechanical deformations. Effectively, CNT fibres behave as yarn-like carbon fibres, with mechanical properties in the high-performance range [2], very high electrical [3] and thermal conductivities and the capability of being processed as staple yarns. This unique combination of characteristic of the material opens routes for new applications of CNT yarns as smart textiles and sensors, as well as for traditional applications such as armour. [1] Y. L. Li, I. A. Kinloch, and A. H. Windle, Science 304 (5668), 276 (2004). [2] K.K.K. Koziol, J. Vilatela, A. Moisala, M. Motta, P. Cunniff, M. Sennett, A.H. Windle, High performance carbon nanotube fiber, Science, 318, 1892 (2007) [3] K. L. Stano, K. Koziol, M. Pick, M. S. Motta, A. Moisala, J. J. Vilatela, S. Frasier and A. H. Windle Int. J. Mater. Form. 1, 59 (2008)

## Poster Board | 136

### NEMS based on relative vibrations of carbon nanotube walls and graphene layers

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At present, a variety of nanoelectromechanical systems (NEMS) that employ carbon layers as movable elements are under development. We consider two types of motion of carbon layers in such systems: a telescopic oscillation with a large displacement of the walls and small vibrations around the commensurate position. In the first case, van der Walls forces saturate at the large wall displacement, resulting in a non-harmonic behavior of the oscillator, while in the second case, the relative vibrations of the walls are approximately harmonic. We perform a multiscale investigation of NEMS based on relative vibrations of carbon layers, starting from study of the interwall potential up to the operation characteristics at macroscopic times. First-principles methods are applied to compute the interaction energy of nanotube walls and graphene layers as a function of their relative position. Then tribological properties of NEMS based on graphene and carbon nanotubes are investigated depending on the parameters and microscopic structure of the system (temperature, length, structure of the walls/layers, etc.) through molecular dynamics simulations. To describe the dynamic behavior of the NEMS at long simulation times we apply a phenomenological model, which is parameterized on the basis of the molecular dynamics results. It is shown that NEMS using telescopic oscillation of carbon layers have limited ranges of phase stability of controlled oscillations due to the non-harmonic character of these systems. In addition, the influence of thermodynamic fluctuations on NEMS operation is examined using the Fokker-Planck equation for the oscillation energy distribution function.

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### Vertically-aligned carbon nanotube membrane filters for oil-water separation

**Cheesung Lee**, *SKKU Advanced Institute of Nanotechnology (SAINT), School of Mechanical Engineering and Department of Energy Science, Sungkyunkwan University* | **Seunghyun Baik**, *SKKU Advanced Institute of Nanotechnology (SAINT), School of Mechanical Engineering and Department of Energy Science, Sungkyunkwan University*

There is great interest in the water-oil separation for industrial and environmental applications. Membrane filters consisting of vertically-aligned multi-wall carbon nanotubes synthesized on stainless steel meshes were fabricated using the thermal chemical vapor deposition method. The nano-scale needle-like tube structure and micro-scale inherent pores of the mesh enhanced both superhydrophobicity, with a water contact angle of 163 degrees, and superoleophilicity with a diesel contact angle of 0. These properties make the membrane selectively permeable to oil while blocking water, resulting in big differences in intrusion pressures and flow rates. The water content in the separated diesel oil was 85.0 ppm. Reference: C. Lee and S. Baik, Carbon48(2010)2192-2197.

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### Cooling of a suspended carbon nanotube by an AC Josephson current flow

**Gustav Sonne**, *University Of Gothenburg, Department of Physics* | **Milton Eduardo Pena-Aza**, *University Of Gothenburg, Department of Physics* | **Leonid Y. Gorelik**, *Chalmers Univeristy of Technology, Department of Applied Physics* | **Robert I. Shekhter**, *University Of Gothenburg, Department of Physics* | **Mats Jonson**, *University Of Gothenburg, Department of Physics; Heriot-Watt University, School of Engineering and Physical Sciences; Konkuk University, School of Physics*

We consider a nanoelectromechanical Josephson junction, where a suspended nanowire serves as a superconducting weak link, and show that an applied DC bias voltage can result in suppression of the flexural vibrations of the wire. This cooling effect is achieved through the transfer of vibronic energy quanta first to voltage driven Andreev states and then to extended quasiparticle electronic states. Our analysis, which is performed for a nanowire in the form of a metallic carbon nanotube and in the framework of the density matrix formalism, shows that such self-cooling is possible down to a level where the average occupation number of the lowest flexural vibration mode of the nanowire is 0.1.

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### Fabrication and characterization of transparent film heater using single-walled carbon nanotube for window application

**Hyunseok Oh**, *Korea Electronics Technology Institute; Yensei University* | **Sunmin Kim**, *Korea Electronics Technology Institute* | **Kwonwoo Shin**, *Korea Electronics Technology Institute* | **Se-Hong Chang**, *Korea Electronics Technology Institute* | **Mun Seok Jeong**, *Gwangju Institute of Science and Technology* | **Jong Hun Han**, *Korea Electronics Technology Institute*

Transparent film heater of low power was manufactured for the window application by spraying single-walled carbon nanotubes (SWCNTs) solution on ionic polymer pre-treated glass substrate. SWCNTs solution was prepared by using SDBS in water and then the aggregated SWCNTs in the solution were almost removed by centrifugation. Simple heating module, which was composed of conductive SWCNT film, electrode, and substrate, was fabricated in order to characterize the performance as a film heater. We applied various metal electrodes (Cr, Au, Ti, and Al) deposited on the substrate by DC sputter before spraying SWCNTs solution. The produced transparent film showed the optical transmittance of 70~85% (at 550nm) and the sheet resistance of 100~500 Ohm/square. In the module test for thermal application, it was observed that the contact resistance between the electrode and the film surface affects total heating efficiency of the film heater severely. Especially, for Al electrode with a low melting temperature, we obtained the excellent transparent film heater with much more reduced ohmic contact resistance when applying DC power of 1~3 kV periodically. After the electric annealing treatment, line resistance of films heater were reduced by maximum 50 % in comparison with untreated film heater. The film heater reaches 120°C with power 0.1W/m2. The patterned film heater was also investigated in order to enhance the thermal uniformity of square-shaped SWCNTs network film because sprayed film on total glass substrate bring commonly non-uniform temperature distribution due to uneven surface resistivity.

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### Graphene-Polyimide composite using easy soluble expanded graphite

**Jong Hak Lee**, *Sungkyunkwan University* | **Xianhui Meng**, *Sungkyunkwan University* | **Dong-Wook Shin**, *Sungkyunkwan University* | **Ji-Beom Yoo**, *Sungkyunkwan University*

ESEG was prepared from a fluorinated graphite intercalation compound (FGIC) – C2F ClF3 containing inorganic volatile intercalating agent ClF3. The interlayer distance of ESEG was 3.64~3.94 Å, which is approximately 17 % higher than that (3.35 Å) of ordinary graphite. This severe expanded state, together with high specific surface area of the ESEG can give us essential material properties for dispersing easily the ESEG in the solution. ESEG suspension prepared in several orgarnic solvents without any surfactant and water with common surfactants using sonication process was subjected to electron microscopy techniques. Analysis showed that, solution consists of exfoliated graphene sheets of thickness 1-2 nm. The ESEG was dispersed sufficiently in NMP, DMAc, DEG, Toluene, DMF, SDBS, DCM, SDS and each solvents had a dispersability of 10, 8.98, 7.28, 6.04, 5.0, 3.78, 1.46, 0.19 micro-g/ml , respectively. This one step exfoliation process of ESEG can allow the low cost mass production of graphene because of the very simple and short process time. In addition, well-dispersed graphene in water and organic solutions have potential use in high-performance, scalable graphene-based applications. We will demonstrate that ESEG could be considered as the preferable reinforcing filler in polymer matrices. Furthermore, without chemical modification, ESEG provide effective anchoring sites for strong bonding with polymers.

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### Influence of Boron Addition on Mechanical Properties of Carbon Nanotubes

**Yoshinori Sato**, *Tohoku University; PRESTO, Japan Science and Technology Agency* | **Kenichi Motomiya**, *Tohoku University* | **Kazuyuki Tohji**, *Tohoku University*

The boron-containing carbon nanotube (CNT) blocks were prepared pressing and heating the CNTs with boron at a given pressure and temperature. Morphology and mechanical properties of boron-doped CNT blocks were characterized using X-ray diffraction (XRD), Raman scattering spectroscopy, scanning electron microscope (SEM), and high-resolution transmission electron microscope (HRTEM). The addition of boron increases in Young's modulus, bending strength, and hardness. The result will be reported in detail and discussed.

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### Mechanical and ElectroProperties of CNT/Polymer Composite with High Aspect ratio CNT

**Toshiyuki Yasuhara**, *Tokyo Institute of Technology* | **Keisuke Ota**, *Tokyo Institute of Technology* | **Naoto Ohtake**, *Tokyo Institute of Technology*

Carbon nanotubes (CNTs) are expected to be a new functional material because they have outstanding mechanical, electrical and thermal properties, compared with conventional carbon fiber. However recent reports indicate that mechanical properties, such as Young's modulus and tensile strength of CNT/polymer composite could not be improved as they are expected. One of the reasons seems that commercial CNTs donft have enough length for reinforcement of mechanical properties at the point of rule of mixture. In order to investigate the effect of CNT length on mechanical properties of composite, CNT aligned along the vertical direction was synthesized by rf plasma CVD method to obtain the uniform length CNT. CNTs of 10nm in diameter, up to 800um in length could be synthesized and the length could be changed by changing the synthesizing time. After melt mixing, tensile test specimens of in-house CNT/polymer composite were fabricated by hot press in a vacuum chamber. As the results of tensile tests, Young's modulus increased by 25% and tensile strength increased by 45% under the condition of 620ƒÊm length and 1wt% CNT loaded. It is found the Young's modulus and tensile strength could be improved by using longer CNT.

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### Effects of physical properties of multiwall carbon nanotube (MWCNT) on electrical conductivity and electrical conduction stability of MWNT nanocomposite

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We report major parameters of MWCNT composites to get the high electrical conductivity. To evaluate these parameters, composite samples were prepared by mixing silicone rubber with different kind of multiwall carbon nanotubes, and the electrical conductivities of the composites were discussed in terms of the waviness, crystallinity and the aspect ratio. It was shown how these physical properties of MWCNT affect the electrical conductivity in the viewpoint of the percolation scaling law. And we also investigate the change of electrical conductivity by static/cyclic heating and its underlying mechanism in the nanotube composite.

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### Thermal boundary resistance in polymer-nanotube composites: a molecular modelling study

**James Elliott**, *University Of Cambridge* | **Sho Hida**, *University of Tokyo* | **Shigeo Maruyama**, *University of Tokyo* | **Junichiro Shiomi**, *University of Tokyo*

We present numerical simulations of the thermal boundary (or Kapitza) resistance of single wall carbon nanotubes (CNTs) embedded in an amorphous polyethylene (PE) matrix. The polymer matrix was first prepared using a coarse-grained lattice model to fully relax the chain conformation near the nanotube-polymer interface, followed by reverse-mapping [1] of an atomistic model. The thermal boundary resistance (TBR) of the CNT-PE system was then calculated via a lumped heat capacity method [2] using the temperature difference between the CNT and PE matrix obtained from non-equilibrium molecular dynamics simulations. The results show that the TBR increases with stiffness of the CNT, indicating elastic heat transport at the interface. On the other hand, TBR decreases with increasing temperature, indicating an increasing contribution of inelastic heat transport. We discuss the implications of these for the production of CNT-polymer composites with more efficient heat transfer at the interfaces. [1] K.R. Haire, T.J. Carver, A.H. Windle, Comput. Theoret. Polym. Sci., 11, 17-28 (2001). [2] C.F. Carlborg, J. Shiomi, S. Maruyama, Phys. Rev. B, 78, 205406 (2008).

## Poster Board | 161

### Electronic and thermal properties of graphene-diamond hybrid structures

**Takahiro Yamamoto**, *The University of Tokyo* | **Takuma Shiga**, *The University of Tokyo* | **Satoru Konabe**, *University of Tsukuba* | **Susumu Okada**, *University of Tsukuba*

We have theoretically investigated electronic and thermal properties of a graphene-diamond hybrid structure consisting of a graphene covalently bonded to the diamond surfaces. In our simulations, the edge structure of graphene at the graphene-diamond interfaces was chosen as Fujita type. The energetics and electronic structures of the hybrid system have been simulated by the ab-initio calculation based on the density-functional theory, and their thermal transport properties have been calculated by the nonequilibrium molecular-dynamics (NEMD) method with Tersoff-Brenner bond order potential. From the ab-initio calculation, we found that the hybrid structure is stable and that the edge state appears at the graphene-diamond interfaces. On the other hand, form the NEMD simulations, we found that the heat flows efficiently from the graphene to the diamond, but it does not flow efficiently in the opposite direction. This is contrary to the fact that the electrical current does not flow from graphene (diamond) to the diamond (graphene). We propose that the graphene-diamond hybrid structure is a potential candidate for novel transmission lines with low energy consumption.

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### Identification of Substitutional Boron in doped Single-Walled Carbon Nanotubes

**Paola Ayala**, *Universität Wien* | **Jason Reppert**, *Clemson University* | **Mandy Grobosch**, *IFW-Dresden* | **Apparao Rao**, *Clemson University* | **Martin Knupfer**, *IFW-Dresden* | **Thomas Pichler**, *Universität Wien*

Substitutional doping of B in single-walled carbon nanotubes (SWCNTs) is a well known functionalization path. Here, it is expected that B atoms substitute C atoms without additional atomic rearrangement, leading to the formation of an acceptor state in the SWCNT electronic structure even at very low B concentrations. These nanotubes have recently gained major attention. Interestingly, superconductivity was reported in thin films containing this material. B substitution in the SWCNT lattice is not necessarily uniform, and the formation of B nano-domains has been considered for a long time. For this reason, quantifying the amount and bonding environments of B in the SWCNT lattice has been challenging, particularly when the doping concentration is below 1at%. In B doped samples similar to those used in this study, EELS studies carried out in a TEM failed to detect the substituted B in the C network. For this reason, B induced changes in the intensity of the RBM and shifts in G' band have been used as indirect proof of substituted B in the SWCNT lattice. Here I will present the direct detection of B in the SWCNT lattice from the core level signal recorded with high resolution x-ray photoelectron spectroscopy. I will show how the corresponding line shape analysis is utilized to identify the different B bonding environments and to correlate the changes in the electronic properties of B doped SWCNTs with Raman spectroscopic studies, elucidating the site selective bonding environments with unprecedented detail even when the B concentration is below 1at%.

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### Influence of purification and covalent functionalization on the electrical conductivity of singlewall carbon nanotube composites

**Iosif Rosca**, *Concordia University* | **Suong Hoa**, *Concordia University*

Single wall carbon nanotubes (SWCNTs) were purified in hydrogen peroxide at room temperature followed by refluxing in hydrochloric acid to remove the iron catalyst. The purified SWCNTs were then functionalized with organic peroxides. The purity and the degree of functionalization of the SWCNTs were assessed by Raman spectroscopy, TGA, TEM, SEM, and EDS. Buckypapers of as-received and functionalized SWCNTs were prepared by membrane filtration of nanotubes dispersed in dimethylformamide. The nanotubes were dispersed in epoxy resin by three-roll milling. The conductivities of the buckypapers and composite plates were measured by van der Pauw method. TEM micrographs evidenced empty capsules formerly filled by the iron nanopaticles, and the EDS analysis confirmed a reduction of the iron content from 5.2 wt% to less than 0.2 wt%. Raman spectroscopy and EDS showed that even during a mild oxidation, functionalization is unavoidable. SEM micrographs evidenced that repeated functionalization with organic peroxide significantly reduces the bundle diameter, fact that improved the dispersion in epoxy resin, but resulted in a lower electrical conductivity of the composite.

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### Functionalization of Double-Walled Carbon Nanotubes

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Double-walled carbon nanotubes (DWNTs) have gained increasing attention because of their unique structure. The potential applications in various fields have been explored, such as field-effect transistors, atomic force microscope (AFM) tips, filaments, energy conversion materials, and resistors. However, the poor insolubility of DWNTs in most common solvents severely impedes their manipulation and application. Here, we report that both covalent and non-covalent functionalization can afford a large increase of the water solubility of DWNTs. In the covalent approach, DWNTs have been modified with diazido-terminated polyethylene glycol (PEG) and azido-terminated PEG monomethylether by cycloaddition reaction. Both PEGs endowed DWNTs with good water solubility. In the non-covalent approach, we used several proteins to disperse DWNTs. By adjusting the conditions, stable aqueous suspensions of debundled DWNTs were achieved. The advantages of these two approaches are discussed.

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### Dispersion of Single Walled Carbon Nanotubes using Carbazole and Fluorene based Polymers

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Separation techniques for single walled carbon nanotubes (SWNTs) have become an important research field over the last several years, because present synthesis methods do not allow the growth of nanotubes of one length, diameter, chirality, electronic type (metallic or semiconducting) and free of byproducts. In this current work, a variety of conjugated polymers based on carbazole and fluorene units has been synthesized and used to obtained dispersions of SWNTs in organic media after ultrasonic treatment. Moreover, these suspensions were subjected to density gradient centrifugation to obtain an enrichment of (n,m) species depending on the polymers. Evidence is provided by optical absorbance and photoluminescence excitation spectra. In addition we perfomed MD simulations to further confirm our experimental findings. Using all-atom simulations we elucidate the origin of the difference in selectivity by the propensity of the different polymers selectively associate with tubes of similar radius, but different chiral index. These findings suggest that chemical screening of closely related polymers may lead to selective salvation of different families of carbon nanotubes. References N. Stürzl, F. Hennrich, S. Lebedkin, M. M. Kappes, J. Phys. Chem. C 113 (2009), 14628.

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### N-type doping of single-walled carbon nanotubes with organic molecules

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We carried out the chemical modification of single-walled carbon nanotubes (SWCNTs) random network by Tetramethylpyrazine (TMP) and N,N,N¡Ç,N¡Ç-Tetramethyl-p-phenylenediamine (TMPD) organic molecules dissolved in THF. Adsorption and intercalation of organic amine molecules in bundled SWCNTs lead to the typical n-type doping like alkali metals. Chemical modification involves physisorption or chemisorption of atoms or ions or molecules on the wall of the SWCNTs and also migration them into the bundle of SWCNTs. The functionalization of SWCNTs has been studied using different kinds of structures of amine. Raman spectra show systematic changes of the typical Raman modes with the concentration of doping molecules, which indicates the n-type doping into the SWCNTs. The metallic feature in the G-band reveals prominent interaction of the SWCNTs with TMP and TMPD, which provides evidence of charge transfer from organic molecules to the SWCNTs. Among the two n-type dopants, the TMPD shows stronger changes in the XPS and the Raman spectra compared with TMP, which clearly demonstrate the difference in the structure of the dopant molecule is reflected in the doping effect. In the XPS spectra, the peak position of C 1s observed at 284.4 eV for the sp2 carbon in pristine sample is shifted by 0.3 eV to the higher binding energy after chemical treatment. We observed that both the TMP and TMPD increase the sheet resistance of the SWCNT network. Finally, we also confirm the n-type semiconducting behavior from the back-gated TFT devices after doping TMPD into the SWCNTs network.

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### Wafer-Scale Carbon Nanotube Alignment and Interaction on Hydrophobic and Hydrophilic Surfaces

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Background Using single-walled carbon nanotubes (SWNTs) for transparent electrode and transistor applications requires top-down control of their length, chirality, placement, and alignment. We develop a wafer-scalable method for electronically pure

SWNT alignment and placement by meniscus action. Design In this technique, we form a meniscus between two surfaces with an aqueous solution of surfactant-coated SWNTs. We employ a glass capillary array as the top surface, filling them with SWNT solution. After meniscus formation, we drag the meniscus across the substrate with a translation platform, aligning SWNTs on the surface. Results On hydrophilic surfaces like SiO2 and Si3N4, we note that SWNT alignment occurs parallel to the drag direction. With constant timestep Monte Carlo simulation, we find that alignment occurs through mechanical torque by surface roughness pinning. Atomic force microscopy (AFM) analysis shows that for SiO2 the SWNTs align at angles 7.99±10.92°, 5.80±12.97°, and 5.35±17.2° for meniscus velocities of 203, 272, and 543 µm/s, respectively, indicating good alignment in the drag direction. On hydrophobic surfaces like H-Si(111) and positive-tone photoresist, SWNTs longer than 800 nm align perpendicular to the drag direction. We attribute this to hydrophilic-hydrophobic surface energy minimization. In our process, we can place SWNTs in densities of up to ~30 SWNTs/µm$^2$, with the density exponentially dependent on the number of meniscus passes. Conclusion Understanding the SWNT interaction on hydrophobic and hydrophilic surfaces allows wafer-scale control of SWNT alignment and placement. We are developing SWNT crossbar memory structures and field-effect transistors with the technique.

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### Selective dispersion of carbon nanotubes in polyfluorene solutions studied by optical spectroscopy and molecular dynamics

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The preparation of single walled carbon nanotubes (SWNT) dispersions in several solvents, and using several encapsulating agents, has allowed the study of the properties of individual nanotubes. These dispersions can further be used to separate suspended SWNT by diameter, for instance by ultracentrifugation in a density gradient. It was recently demonstrated that conjugated polymers from the polyfluorene family are able to wrap selectively in nanotubes having high chiral angles, especially when toluene is used as solvent. In the present work we report on the photophysical properties of SWNT suspensions in toluene solutions of poly[9,9-dioctylfluorenyl-2,7-diyl](PFO). Steady-state and time-resolved photoluminescence spectroscopy in the near infrared and visible spectral regions are used to study the interaction of the dispersed SWNT and the wrapped polymer. Molecular dynamics simulations of the PFO-wrapped nanotubes in toluene were carried out to assess the conformation of these systems. The simulated fluorescence spectra in the visible region were obtained by the quantum chemical ZINDO-CI method, using a sampling of structures obtained from the dynamics trajectories. We were able to show that PFO chains adsorb in SWNT surface in basically two conformations. The polymer chains are either aligned along the nanotube axis, where chirality has a minimal effect, or the polymers form helical structures, where a preference for high chiral angles is evidenced. Toluene affects the polymer structure favoring the helical conformation. The most stable hybrid system is the PFO-wrapped (8,6) nanotube, in agreement with the experimentally observed selectivity.

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### Surface modification of MWCNTs in the afterglow of a cold atmospheric plasma jet

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Improving the properties of polymers by the addition of carbon nanotubes (CNTs) requires an efficient dispersion and alignment of the CNTs in and interfacial adhesion to the matrix. Surface modification of CNTs is one possibility to influence these three factors. Oxidative functionalization is frequently the first step for further chemical surface modification of CNTs and is typically performed by using strong inorganic acids. We report on the development of a plasma process that modifies the CNT surface in the relaxing afterglow of a non-thermal atmospheric pressure plasma jet. The plasma process can be easily combined with the industrial CVD synthesis of MWCNTs and reduces drastically the amount of waste typically encountered in acidic treatments. In addition, the process requires very short reaction times (milliseconds) and can be scaled up for high throughput (several kg/day). As XPS analysis shows, the plasma treatment incorporates about 8 at% of oxygen into the CNT surface. The formation of different oxygen-containing functional groups is observed, while the degree of functionalization can be controlled by the treatment time. TGA and Raman spectroscopy are used to study the change of CNT structure and the formation of defects. Both seem to be only slightly affected by the plasma treatment. The improvements in dispersability are shown by contact angle and sedimentation measurements. The improvements in matrix adhesion are studied by characterizing CNT/epoxy nanocomposites. These results indicate that the atmospheric plasma process can provide an attractive alternative to wet chemical processing.

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### Carbon nanotubes-photosystem I and –hydrogenase biohybrids for energy devices

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Biohybrids take advantage of the evolutionarily optimized function of enzymes in the design of efficient devices for applications such as diagnostics, catalysis or self-assembly. Focusing on alternative energy devices, we chose two redox enzymes: photosystem I (PSI) for photovoltaic cells and hydrogenases for hydrogen fuel cells. The proteins were coupled to carbon nanotubes (CNT)s as nanoelectrodes to collect electrons. PSI is one of the main light harvesting complexes involved in photosynthesis in plants, algae and cyanobacteria. We first incorporated PSI from cyanobacteria into photosensitive CNT transistors to test their stability in electronic, dry devices. The phototransistors showed good robustness and a high sensitivity to light (<10mW/cm$^2$). Covalent coupling of PSI onto CNTs is now under way to control the protein orientation and optimize electron transfer to the nanotube for photocurrent collection. Hydrogenases catalyse hydrogen oxidation in numerous bacteria with a very high activity in solution, which makes it worth testing them as an alternative to platinum catalysts. Covalently coupled hydrogenase-CNT biohybrids were prepared and characterized by AFM, XPS and cyclic voltammetry. The proteins were coupled through their carboxyl groups to allow direct electron transfer from their active site to the CNT. Integration on fuel cell Gas Diffusion Layer is under way to evaluate their catalytic efficiency in a realistic fuel cell system. In spite of their notorious fragility, the proteins are shown to keep their functionalities once integrated with CNTs and they could provide interesting components for energy production.

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### Designing Density Gradient Ultracentrifugation Recipes for Desired Separation of Single-Walled Carbon Nanotubes

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The density gradient ultracentrifugation (DGU) method adapted to SWNTs is considered one of the most promising and effective for achieving good SWNT selectivity. We used this method to sort surfactant-dispersed single-walled carbon nanotubes (SWNTs) by their diameters or electronic types. As to diameter separation, a controllable multicolored expansion was obtained in which the average SWNT diameter increased in each successive colored layer. By adjusting the concentration and types of surfactants, as well as choosing a suitable density gradient profile, this expansion can be further expanded or contracted. Furthermore, tuning the surfactant concentrations can result in electronic type separation, or even a simultaneous isolation of (6,5) nanotubes in addition to separation by electronic type. Investigating the experimental conditions yielding these different results allowed us to investigate the mechanism behind this surfactant-assisted separation. We find that the addition of bile salts such as sodium deoxycholate (DOC) or sodium cholate (SC) are used in combination with sodium dodecyl sulfate (SDS), their hydration conditions,activation energies with SWNTs, and surrounding environments will determine how they adsorb onto the nanotube surfaces, which will further determine the density of the formed surfactant-SWNT micelles. This model can not only explain these results but also make predictions based on the DGU starting recipes.

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### Molecularly engineered “peapods”: tuning the electro-optical response of SWNTs

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Despite carbon nanotubes are characterized by high electrical and thermal conductivity, they do not absorb light in the visible region (350-800 nm) extensively. In order to exploit single-walled carbon nanotubes (SWNTs) as functional materials in such application as photoelectrochemical cells, photodetectors and organic light-emitting diodes, it is necessary to design supramolecular structures responsive to visible light. Indeed, the engineering of the properties of carbon nanotube is possible by encapsulating organic photoactive molecules to obtain supramolecular entities, usually referred as “peapods”, that combine the electrical and thermal conductivity of SWNTs and the optical properties of the guest. In this work we encapsulated suitable polycyclic aromatic hydrocarbons (such as pyrene and coronene) in shortened purified SWNTs by nano-extraction, vapor-phase technique and using supercritical carbon dioxide. We studied the novel peapods by means of steady-state and time-resolved UV-vis spectroscopy, Raman spectroscopy, thermogravimetric analysis, and HRTEM. All the results point out that we did succeed in the encapsulation processes. Moreover, the spectral fingerprints of the peapods are markedly different from those of the isolated compounds, suggesting an efficient guest-host coupling to form interacting supramolecular assemblies. In conclusion, we were able to design, synthesize and characterize novel SWNT-based peapods to be incorporated in functional materials exhibiting improved electro-optical response over the visible spectrum.

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### Properties of Phenyl- and Methylene- Functionalized Carbon Nanotubes

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Covalent functionalization of carbon nanotubes (CNT) appears nowadays as one of the most important chemical tools enabling the processing, manipulation and assembly of CNT from solution. However, little is known about the effect of the chemical reaction on the electronic properties of the CNTs and about the thermal stability of the functionalized derivatives. Here, we compare the repercussions and the stability of monovalent and bivalent adducts grafted on CNT. The first case studied involves phenyl adducts attached by a covalent bonding to a single site of the sidewall. The second case involves methylene adducts that bridge two carbon sites of CNT. We analyzed the decrease of conductivity and light absorption induced by these functionalizations. We also determined the thermal stability of the CNT derivatives using temperature desorption spectroscopy (TDS). The results show that the methylene moities are detached from the sidewalls at ~500 K while, under the same experimental conditions, the phenyls are removed at ~600 K. In addition, we observed no influence from the helicity and diameter distributions of the different samples of CNT studied (mean diameter: 0,81 nm versus 0,93 nm). Moreover we proved that the detachment of the phenyl adducts occurs through a phenyl-phenyl coupling at the sidewall. The advantages of the covalent functionalization for applications in nanoelectronics will be discussed.

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### High-Yield Purification of Double-Walled Carbon Nanotubes for Optical Modulation

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Transparent and conductive thin films were prepared from purified double-walled carbon nanotubes (DWNTs). Purification of the as-received soot was achieved in a two-step process: The key step is a high temperature endothermic oxidation in a pure CO2 gas flow according to the Boudouard reaction which is combined with a standard reflux in concentrated nitric acid. This treatment provides fast oxidation of amorphous carbon and removal of other impurities without affecting the carbon nanotubes. Parameterization of the high temperature reaction was explored to selectively remove single-wall NT and highly-damaged DWNTs. AFM, TEM, XPS, UV-vis-IR absorption and Raman spectroscopy analyses reveal that the films are composed of high quality DWNTs (micrometer long nanotubes, very low impurity concentration, high Raman IG/ID ratios). The films were then used as electrodes for light modulating devices using a polyelectrolyte to induce charge injection doping. Those devices give an effective modulation of the absorption of the first optical transition of the semiconducting outer walls.

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### Biotin molecules on the surface of nitrogen-doped carbon nanotubes enhance the anchoring and formation Ag nanoparticles

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A simple, efficient and innovative method for anchoring Ag nanoparticles on the surface of nitrogen-doped multi-walled carbon nanotubes (CNx-MWNTs) is reported. The process involves the attachment of an important bio-molecule, biotin

(C10H16N2O3S), on the surface of CNx-MWNTs, which then acts as a reducing agent of AgNO3, and causes the efficient anchoring of Ag nanoparticles. Silver nanoparticles with average diameters ranging from 1-3 nm were found strongly attached to CNx-MWNTs. A comparative study using pristine MWNTs (undoped) and acid treatment MWNTs, revealed that the Ag particles anchored to the tubes exhibited much larger diameters and less anchoring efficiency. The method involved the reaction of biotin-CNx MWNT mixtures with AgNO3 at room temperature. The samples were characterized using SEM, HRTEM, Raman spectroscopy, AFM, X-ray diffraction and thermogravimetry. In order to elucidate the mechanism whereby Ag nanoparticles strongly bind to the surface of the CNx nanotube, we carried out density functional calculations that revealed the existence of a covalent bond established between the biotin molecule and the nitrogen doped carbon nanotube through the oxygen atom, leaving the sulfur atom exposed to the other end of the biotin molecule. This sulfur atom is expected to interact strongly with the Ag atoms, and even be able to reduce AgNO3. Finally, we experimentally demonstrated that the Ag-biotinated CNx-MWNTs could be used as efficient sensors for detecting CS2 vapors. We believe that the synthesis of these biotinated CNx-MWNTs could also be used in other biotechnology processes in which biotin is vital, and further investigations are currently underway.

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### Theoretical study on the interactions between nitrogen- and boron-doped carbon nanotubes and glutamic acid

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The interactions established between metallic (10,10) pure carbon single-walled (SWNT), boron-doped (CBx) and nitrogen-doped (CNx) carbon nanotubes with glutamic acid molecules, are assessed using density functional theory (DFT) and semi-empirical approaches. The three systems (SWNTs, CBx and CNx) are simulated using three different configurations: pristine, oxidized (functional COOH groups attached to the nanotubes wall), and functionalized with glutamic acid at the oxidized sites. The results indicate a strong electronic localization occurring on the functionalization points of the doped nanotubes (CBx and CNx) with stabilized glutamic acid molecules on their surface. In addition, the observed significant changes in the systems' densities of states (DOS) shows efficient sensing properties through the biomolecule activity, suggesting their use as biomarkers and biosensors.

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### Synthesis of nitrogen doped carbon nanotubes by growth methodes

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We synthesize the nitrogen doped (N-doped) carbon nanotubes by plasma enhanced chemical vapor deposition (PE-CVD) and thermal chemical vapor deposition (T-CVD), and investigated by synchrotron X-ray photoelectron spectroscopy (XPS) ,Extended X-ray Absorption Fine Structure (EXAFS) and Raman microscopy. In this paper, the experimental observation of nitrogen incorporation in multiwalled carbon nanotubes (MWCNTs) by growth methode is reported. Nitrogen source of N-CNT was doped using NH3. XPS, EXAFS and Raman microscopy were used to assess quantitatively the compositional and structural properties of the N-doped carbon nanotubes (N-CNTs). XPS analysis indicates a shift in and broadening of the C 1s spectra track with increasing disorder induced by selective nitrogen doping. N 1s XPS spectra show three principle types of nitrogen coordination (pyridinic, pyrolic, and quaternary). N-CNT was confirmed berry different by measurements according to growth methode. N-CNT will be applied to an electrode of the fuel cell to establish the foundation of the hydrogen energy system.

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### Transmission electron microscopy studies of the orientation and structure of Fe, Co and Ni nanoparticles inside carbon nanotubes and nanofibers

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Background: Synthesis of carbon nanostructures on metal catalyst is of great importance both in fundamental and applied physics. It is already well known that orientation relationships between the crystal lattice of the catalyst nanoparticle and the carbon layers segregating on it play key role in nanostructure growth. The interaction between the carbon layers and the nanoparticle directly affects its shape, orientation and defects. Design: The goal of the present study is understanding of carbon nanotube/nanofiber interaction with catalyst nanoparticle in terms of their mutual crystallographic orientation and reshaping of the particle. Results: Carbon nanotubes obtained by CVD and also inside the high isostatic pressure apparatus on metal catalyst (Fe, Co and Ni) were investigated in details in transmission electron microscope JEM-2010. The nanotubes contain the nanoparticles of the abovementioned metals. Some of them are catalyst particles while the others were drawn into the nanotubes during the growth process. Many of them were subjected to deformation and twinning due to the interaction with nanotube walls. Shape, crystallographic orientation and defects of these metal nanoparticles were examined. Conclusion: It is determined that particles with both b.c.c. (Fe) and f.c.c. lattices (Fe, Co, Ni) have the same sets of orientations along the nanotube axis: [100], [110], [111] and [112]. Twins in twinned particles have additional set of orientations which correspond to the orientation relationships between the twinned and the origin lattices. The shape, the orientation and the defects of the nanoparticles are considered taking into account the model of the nanotube epitaxial growth.

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### Characterization of graphene interlayer interaction using cup stack carbon nanotubes

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Cup stacked type carbon nanotube (CSCNT), due to its structure with graphene edge appearing in the sidewall, is an interesting material that can be regarded as an intermediate structure between cylindrical nanotube and stacked graphene sheets. By means of in-situ electric property measurements of individual CSCNT in the transmission electron microscpe, we found the change in the electric conductivity during application of axial force to the CSCNT. We consider this to be due to the interlayer interacation whithin the CSCNT, and will be detailed at the conference.

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### Imaging the operation of a carbon nanotube charge sensor at the nanoscale

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Carbon nanotubes are of great interest for nanoelectronics applications such non volatile memory elements (NVMEs) or charge sensors [1]. In this work, we identify, using combined transport, scanning probe techniques and atomistic simulations, the fundamental mechanisms of NVMEs based on individual

CNTFETs. The response of NVMEs is investigated using a scanning force techniques such as Electrostatic Force Microscopy (EFM) and Kelvin Force Microscopy (KFM), in order to map charges (down to few electrons) and surface potentials at the nanoscale in the nanotube environment [2,3]. We demonstrate operating devices with threshold voltages shifts opposite to conventional gating and unchanged hysteresis [4]. The former effect is quantitatively understood as the emission of a delocalized image charge pattern in the nanotube environment, in response to local charge storage, for which we propose a simple model for charge sensing, based on the redistribution of the nanotube image charges. This model could also be extended for e.g. gas sensing or biosensing. The latter effect demonstrates the dominant dipolar nature of hysteresis in CNTFETs - based on molecular species in the nanotube environment - rather than on charges at the nanotube/SiO2 interface. [1] Gruneis et al., NanoLetters 7, 3766 (2007) [2] Zdrojek et al., PRB 77, 033404 (2008) [3] Brunel et al, APL 94, 223508 (2009) [4] Brunel et al, submitted

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### Potential Barriers of Carbon Nanotube FETs Investigated by Scanning Gate Microscopy and AFM Potentiometry

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A carbon nanotube field effect transistor (CN-FET) using single wall carbon nanotubes (SWNTs) is one of the most promising applications in next-generation electronics. The CN-FET characteristics strongly depend not only on the electronic state of the SWNT itself but also on the potential barriers corresponding to the metal-SWNT contact interfaces or some intrinsic defects. The development of a method for analyzing these local electronic states on a nanometer scale is indispensable for thorough understanding of the SWNT channel conduction. In this study, we have investigated the electronic states of CN-FETs in working condition by newly developed scanning gate microscopy (SGM) and atomic force microscope potentiometry (AFMP), to which we applied the point-by-point measurement technique. Since SGM image contrast reflects the change in the channel current caused by the local electric field applied by the AFM tip, SGM directly tells you the positions of local potential barriers and their electrical characteristics. On the other hand, the local resistance on the channel can be estimated by the surface potential distribution obtained by AFMP. We first fabricated CN-FETs, in which the isolated SWNT was connected to two Pd electrodes by dielectrophoresis using a (6, 5) enriched solution, prepared by the density gradient ultracentrifugation separation technique. The potential barriers of the CN-FETs were investigated by SGM and AFMP in vacuum. We successfully visualized the potential barriers corresponding to intrinsic defects in the channel and the Schottky barrier at the contact interface. The result showed the channel current was controlled at the potential barriers.

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### Temperature dependence of electrical resistance of transparent heater made of single-walled carbon nanotubes

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We experimentally studied thermal behavior of transparent film heater (TFH) using single-walled carbon nanotubes (SWCNTs). We fabricated the TFH by using the spray coating method. We investigated the temperature dependence of the electrical resistance of the TFH in terms of Joule and external heating in various gas environments. Test results show that the effect of the electrical current through the TFH on the temperature dependence of the electrical resistance is not important and that the humidity and the degree of vacuum significantly affect the shape of the resistance-temperature curve. We discussed physical meanings underlying the experimental results and how to make use of the findings. This study provides useful information on the thermal behavior of the transparent conducting films made of SWCNTs.

## Poster Board | 237

### Topological defects in carbon nanohorns: neutron and X-ray diffraction studies

**Andrzej Burian**, *A. Chelkowski Institute of Physics, University of Silesia, Poland* | **Aleksander Brodka**, *A. Chelkowski Institute of Physics, University of Silesia, Poland* | **John Dore**, *School of Physical Sciences, University of Kent, UK* | **Alex Hannon**, *Rutherford Appleton Laboratoty, UK* | **Katsumi Kaneko**, *Chiba Universit, Japan*

The structure of single-wall carbon nanohorns produced by laser ablation at room temperature without a metal catalyst has been studied using pulsed neutron, X-ray diffraction and molecular dynamics. The collected diffraction data have been converted to a real space representation in the form of the pair correlation function via the sine Fourier transform. For computer generated models consisting of a nanocone with the cone angle approximately 20o and single-wall carbon nanotubes of the perfect hexagonal structure about 350 Å in length and 20 Å, 25 Å and 30 Å in diameter the computed diffracted intensities and pair correlation functions are in reasonable agreement with the experimental data. For larger nanohorns of 50 Å diameter features of the experimental pair correlation function cannot be reproduced using the model in which all carbon atoms are arranged into six membered rings and Stone-Wales, mono-vacancy and di-vacancy type defects have been introduced to fit the experimental data. All the models have been relaxed using the molecular dynamics method with the reactive empirical bond order potential (REBO2) for carbon-carbon interactions. The best fit to the experimental data has been obtained for the model with the Stone-Wales defects although the presence of the mono- and di-vacancies cannot be completely ruled out. The proposed procedure is expected to be useful when production of carbon nanomaterials on a mass scale for a wide variety of industrial applications is of importance.

## Poster Board | 239

### Photoconductivity of multi-wall and single-wall Boron-Nitride Nanotubes

**Sylvain Maine**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France* | **Gurvan Brasse**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France* | **Aurélie Pierret**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France* | **Périne Jaffrennou**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France* | **Cyrielle Roquelet**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France* | **Brigitte Attal-Trétout**, *ONERA - Département Mesures Physiques (DMPH), France* | **Annick Loiseau**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France* | **François Ducastelle**, *ONERA - Laboratoire d'Étude des Microstructures (LEM), UMR 104 Onera-Cnrs, France*

Boron-Nitride (BN) nanotubes (NTs) have a large potential for optical applications, especially for the development of UV light sources. The optoelectronic properties of such wide band gap semiconductors are not well known, especially the energy band gap values and the energetic fine structure of the forbidden band near the band edge. Here, an original method is proposed to study the UV photoconductivity of single wall BNNTs, multiwall BNNTs and hBN crystals. The experimental setup is composed of a deuterium lamp equipped with a condenser, an UV-VIS monochromator followed by a Cassegrain objective to excite the sample. The samples are deposited on an electronic device formed of 80 nm thick interdigited Pt electrodes on a silica-on-silicon substrate. The induced photocurrent is measured thanks to tungsten tips connected to the electrodes pads. The experiments have provided response of hBN crystals, MWBNNTs and SWBNTs. A calibration of the setup has then been achieved using an UV photomultiplier to correct the experimental data, in order to accurately measure energy band gaps. Eventually a fine structure is highlighted near the band edge and is correlated with microphotoluminescence spectra of the same samples.

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### Raman spectroscopy investigation of the early growth stages of aligned multi-walled carbon nanotubes

**Périne Landois**, *CEA-Saclay Laboratoire Francis Perrin, France* | **Celia Castro**, *CEA-Saclay Laboratoire Francis Perrin, France* | **Mathieu Pinault**, *CEA-Saclay Laboratoire Francis Perrin, France* | **Martine Mayne-L'Hermite**, *CEA-Saclay Laboratoire Francis Perrin, France* | **Nedjma Bendiab**, *Institut Néel CNRS/UJF,France*

The control of synthesis process of carbon nanotubes (CNT) is particularly important in order to tune their physical and chemical properties. This will be possible if growth mechanisms of CNT are determined and understood. The different questions commonly reported are the nature, structure and state of the catalyst particles, as well as the structural changes of both catalyst particles and CNT during CNT nucleation and growth steps. To answer these open questions, Raman spectroscopy has been performed on aligned multi-walled CNT (MWNT) during the first steps of the growth. We have compared the effect of a standard cooling step (inertia of the oven) to a quenched cooling step, on the iron-based phases. Identification of different iron-based phases such as iron oxides ($Fe_2O_3$) and carbide ($Fe_3C$) and progressive structural organization of carbon toward CNT structure will be presented and discussed. Moreover, we demontrate that Raman mapping is possible on such samples and that there is a relation between iron-based phases and carbon structures.

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### Encasing Single-Walled Carbon Nanotubes with Solvent Microenvironments

**Kirk Ziegler**, *University Of Florida* | **Carlos Silvera Batista**, *University Of Florida* | **Randy Wang**, *University Of Florida* | **Wei-Chiang Chen**, *University Of Florida* | **Cheng-Ying Lin**, *University Of Florida*

Surfactants are typically used to disperse single-walled carbon nanotubes (SWNTs) in aqueous suspensions. The hydrophobic end of the surfactant shell attaches to the sidewall while the hydrophilic end extends into the aqueous phase, providing the needed repulsive barrier to disperse the SWNTs. Here, we will show that mixing aqueous SWNT suspensions with immiscible solvents swells the hydrophobic region between the surfactant and the nanotube. Both spectroscopy and SANS studies show that small regions of the solvent encase the SWNTs. These emulsion-like microenvironments surrounding the SWNTs provide an ability to study the environmental effects on SWNT fluorescence emission energy and intensity. These solvent shells can also deliver hydrophobic molecules onto the sidewall of the nanotubes, enabling organic chemistry, such as polymerization reactions, to be conducted in a microreactor encasing individual SWNTs. The solvent shells surrounding the SWNTs are often reversible once the solvent evaporates. However, some surfactant-solvent systems show permanent changes to the NIR fluorescence emission intensity after exposure to the organic solvent. These differences are attributed to surfactant reorganization, which improves nanotube coverage and decreases exposure to quenching mechanisms from the aqueous phase.

## Poster Board | 245

### Effect of TiO2 nanoparticles decoration on thermal properties of multi-wall carbon nanotubes: a Raman investigation

**Carla Verissimo**, *Center for Semiconductor Components, University of Campinas - UNICAMP, Campinas, SP, Brazil* | **Angela M. O. de Zevallos Márquez**, *Instituto de Fisica Gleb Wataghin, University of Campinas - UNICAMP, Brazil* | **Maria J. S. P. Brasil**, *Instituto de Fisica Gleb Wataghin, University of Campinas - UNICAMP, Brazil* | **Fernando Iikawa**, *Instituto de Fisica Gleb Wataghin, University of Campinas - UNICAMP, Brazil* | **Alireza Abbaspourrad**, *Center for Semiconductor Components, University of Campinas - UNICAMP, Campinas, SP, Brazil* | **Stanislav Moshkalev**, *Center for Semiconductor Components, University of Campinas - UNICAMP, Campinas, SP, Brazil* | **Oswaldo L. Alves**, *Laboratório de Química do Estado Sólido – LQES, Instituto de Química, University of Campinas - UNICAMP, Brazil*

Potential applications for carbon nanotubes (CNTs) extend to a large number of areas such as electronics, sensors, catalysts and energy storage. In the last years, novel hybrid materials consisting of CNTs decorated with nanoparticles of different materials have been proposed as an alternative to modify and control CNTs properties in order to adjust them for specific applications. Herein, we have investigated the effects of decorating multi-wall CNTs with $TiO_2$ nanoparticles. Purified CNTs were treated with nitric acid to promote a mild oxidation and then submitted to a decoration process. An in situ growth of $TiO_2$ nanoparticles was performed using titanium tetrachloride as the metal precursor in hydrolysis reactions under controlled pH values. Decorated CNTs were characterized by scanning and transmission electron microscopy. We observed the formation of $TiO_2$ aggregates with cauliflower-like shapes with relatively large dimensions (bigger than 100 nm) and small individual $TiO_2$ nanoparticles (smaller than 10 nm) directly attached to the CNTs surfaces. A detailed Raman spectroscopy study was performed in pristine and in a series of decorated CNTs obtained using slightly different growth procedures. Depending on the decoration process conditions, crystalline $TiO_2$ nanoparticles with anatase structure are observed by Raman spectroscopy and their signal is also analyzed. We demonstrate that the attached $TiO_2$ nanoparticles strongly affect the thermal properties of the nanotubes, as revealed by differentiated reactions to laser heating. This is an important result for practical applications, since heat dissipation is a fundamental point for the development of various CNTs based devices.

## Poster Board | 249

### DSC Studies of Functionalisation of SWCNTs

**Keith Paton**, *Thomas Swan & Co. Ltd.* | **Marcelo Motta**

Nitric acid oxidation has been well established as an effective method of both purifying and functionalising carbon nanotubes, both single and multi-walled. It has recently been proposed that rather than reacting directly with the nanotube surface itself, the acid treatment generates amorphous carbon debris, and that it is this that is then functionalised[1]. To the best of our knowledge however, there has been no systematic study to date of the heat of reaction during this process. This heat of reaction is an important parameter as such processes are scaled-up to industrial production. The heat evolved during the reaction will be affected by parameters such as amorphous carbon content, defects in the tube structure and concentration of acid used, as well as residual metal content from synthesis. Differential scanning calorimetry (DSC) allows the enthalpy of reactions to be studied with great accuracy. In the present work we have carried out a DSC study of both the nitric acid functionalisation, and the thermal desorption of functional groups from single-walled carbon nanotubes. A clear exothermic peak at ~52°C is observed during acid functionalisation, the position of which is invariant with amorphous carbon content. The thermal desorption of functional groups has also been studied using tubes that have previously been acid functionalised. By studying the behaviour of acid treated tubes that have subsequently undergone a dilute basic wash, the hypothesis of functionalisation of amorphous carbon has been tested. [1] Fogden et al, Chem. Phys. Lett. 460 (2008) 162-167

## Poster Board | 250

### Raman Spectroscopy of isolated single-walled carbon nanotubes in a device configuration

**Asaf Avnon**, *Freie Universitaet Berlin* | **Cinzia Casiraghi**, *Freie Universitaet Berlin* | **Abbes Tahraoui**, *Paul Drude Institute* | **Shu- Pei Oei**, *University of Cambridge* | **William Milne**, *University of Cambridge* | **Stephanie Reich**, *Freie Universitaet Berlin*

Raman spectroscopy is a very powerful technique to investigate single walled carbon nanotubes (SWNT). It can identify a nanotube, and provide information on the diameter, the amount of defects and electronic properties of a SWNT. Here we measured the Raman spectra of isolated SWNT in a device configuration. The SWNTs were grown by chemical vapor deposition (CVD) on a silicon/silicon oxide substrate and contacted by e-beam lithography. We performed a systematic analysis of the first-order Raman spectrum by measuring nine nanotube-based devices. Further results on the radial breathing mode and the second-order Raman spectrum are presented.

## Poster Board | 252

### Bending modulus of freestanding carbon nanotubes

**Henrik Jackman**, *Physics and Electrical Engineering, Karlstad University, Sweden* | **Pavel Krakhmalev**, *Mechanical and Materials Engineering, Karlstad University, Sweden* | **Krister Svensson**, *Physics and Electrical Engineering, Karlstad University, Sweden*

The bending modulus of carbon nanotubes (CNTs) has previously been studied by measuring the amplitude of their intrinsic thermal vibrations [1], exciting vibrations to their fundamental frequency [2], and by static deflections of CNTs supported by a substrate [3]. These studies indicate that the bending modulus depends on the diameter of the CNT, while the bending modulus should be a material constant which is independent on the dimensions of the structure. In previous studies, [1] and [2], no force measurements have been made, and in study [3] the force measurements were made on substrate supported CNTs. To our knowledge no direct force measurements have yet been performed on freestanding CNTs. Here we have used a custom made AFM inside an SEM to perform direct force measurements on individual, freestanding, multiwalled carbon nanotubes (MWCNT). By pushing a MWCNT against a piezoresistive cantilever the spring constant of the MWCNT can be obtained. From the SEM one obtains the dimensions of the MWCNT and the bending modulus can be calculated using simple beam theory. Our preliminary data for the bending modulus of large diameter MWCNTs ($D > 35$ nm) were in the range of 10-100 GPa in agreement with previous observations using vibrational analysis [2]. [1] M. M. J. Treacy, T. W. Ebbesen, and J. M. Gibson, Nature 381, 678-680 (1996). [2] P. Poncharal, Z. L. Wang, D. Ugarte, and W. A De Heer, Science 283, 1513-1516 (1999). [3] E. W. Wong, P. E. Sheehan, and C. M. Lieber, Science 277, 1971-1975 (1997).

## 12:30-14:00 Poster take-down (for Poster Sessions 4-6)

# AUTHORS INDEX

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