

Seventeenth International Conference on the Science and Application of Nanotubes and Low-Dimensional Materials - NT16

Program for Sunday, August 7 th 2016	
12:30 - 13:00	Special Talk: David Tomanek <i>My life with the nanotube</i>
13:15 - 14:30	Tutorial Talk: Georg Kresse <i>Theoretical Spectroscopy: GW and BSE, an introduction for non-experts</i>
14:30-15:00	<i>Coffee Break</i>
15:00-16:15	Tutorial Talk: Jörg Fink <i>Introduction into current electron-energy-loss and angular-resolved photoelectron spectroscopies</i>
16:30-17:45	Tutorial Talk: Ferenc Simon <i>Magnetic resonance in carbon nanotubes and related structures</i>
18:00-...	<i>Opening Ceremony</i>

SUNDAY

ST: My life with the Nanotube

Tomanek, David (Michigan State University, USA)

My personal involvement with carbon nanotubes (CNTs) started while visiting the lab of late Rick Smalley at Rice during my 1994 sabbatical year. I was impressed by the rapid succession of fundamental discoveries in the field. There was progress in large-scale synthesis, characterization techniques including atomic-level imaging, mechanical toughness and chemical stability, peapods, chirality-dependent ballistic conductance in 1D, record thermal conductivity, and many more. Eventually, I fell in love with the nanotube. To prevent the unique, beautiful material from being forgotten and lose funding like the buckyballs (fullerenes) a few years later, I decided to dedicate my life to forming and continually supporting the community of researchers interested in nanotubes. The goal was to get beyond the curiosity stage to mainstream research and eventually to innovative applications in the consumer market. To promote progress, around 1995 I founded The Nanotube Site, which initially played an important role in defining the community, and organized an International Workshop on the Science and Application of Nanotubes (NT99) in 1999 with the assistance of Richard Enbody, my faculty colleague from the Department of Computer Engineering. My love affair with the nanotube continued with the success of The Nanotube Site and in particular the NT99 workshop. Reaching the "hottest topic status" in early 90's and maintaining it for over a decade indicated that the second goal was reached. With an annual industrial production of hundreds of tons of nanotubes world-wide and their use ranging from performance-enhanced Lithium-Ion Batteries to a mass distribution of CNT touch-screen displays replacing brittle indium-tin-oxide (ITO) during the last decade indicate application potential, the last goal. I continued my involvement with nanotubes until present. To some degrees, I treated the Nanotube conferences like my babies. During the initial years, the number of registered participants exceeded the planned capacity by a factor of two. This was manageable at NT99 in East Lansing, with 120 instead of the planned 60 participants. The following conference, NT01, was planned to accommodate 140 participants at a beautiful location in Potsdam. The large number of applications, close to 300, turned from a blessing to a headache for the organizers. Only half of the applicants could be admitted due to the hard limit, imposed by the hotel capacity at the somewhat remote location. The strong interest in the topic and the conference format held on at NT02 at Boston College. Since then, the number of participants has increased gradually, reaching approximately 900 at NT09 in Beijing.

To reflect the international nature of the research field, the NT03 conference was held at Seoul National University in Korea. By that time, the Asia-Europe-Americas "continent swapping mode" emerged as a pattern. The NT04 conference was held in San Luis Potosi, Mexico. The NT05 conference has been brought back to Europe. NT06 took place in Japan, NT07 in Brazil, NT08 in France, NT09 in China, NT10 in Canada, NT11 in the U.K., NT12 in Australia, NT13 in Finland, NT14 in the USA, NT15 in Japan, NT16 in Austria and NT17 in Brazil.



TUTORIALS

T1: Theoretical Spectroscopy: GW and BSE, an introduction for non-experts



Kresse, Georg (University of Vienna, AUSTRIA)

Georg Kresse is a well-known expert in the development of ab initio density functional methods. His contributions to the enhancement of the numerical algorithms have resulted in one of the most successful density functional theory packages called VASP (Vienna Ab initio Simulation Package), which is presently used by hundreds of academic institutions and many industrial licensees. Simultaneously, he has contributed to a database of PAW potentials covering the entire Periodic Table. Georg Kresse was listed in 2015 by Thomson Reuters among the World's Most Influential Scientific Minds in the field of Physics.

T2: Introduction to current electron-energy-loss and angular-resolved photoelectron spectroscopies



Fink, Jörg (Dresden, GERMANY)

The beginning of Prof. Fink's career is clearly marked by studies of the Mössbauer effect following neutron capture in Gd compounds and on transition metal compounds. From 1978 he embarked on research involving electron spectroscopies, in particular electron energy-loss, angle resolved photoemission (ARPES), and X-ray absorption spectroscopy as well as resonant X-ray scattering. He is a world renowned expert in these fields. In 1994 he took up a full professorship at the Dresden University of Technology and was director of the Institute for Solid State Research at the IFW Dresden. After the official retirement in 2003 he continued to do research at the IFW Dresden, at Ames Lab, and at Helmholtz-Zentrum Berlin (BESSY).

T3: Magnetic Resonance in Carbon Nanotubes and Related Structures



Simon, Ferenc (University of Budapest, HUNGARY)

Professor of the Department of Physics of the Faculty of Natural Sciences at the University of Budapest. Prof. Simon is an expert in Magnetic Resonance applied to Carbon nanostructured materials. His professional development involves periods in the UK (Manchester), France, Switzerland and Austria). He has received significant European Funding for his research in the field: the Marie-Curie Intraeuropean Fellowship and a Reintegration Grant and the ERC in 2010. Ferenc Simon has taken a very active role in education in Physics in Hungary and Austria.

Program for Monday, August 8th 2016

09:00-9:45	Key Note Lecture: Junichiro Kono <i>Progress Towards Single Crystals of Carbon Nanotubes</i>
09:45-10:00	Contributed Talk: Wenshan Li <i>Chiral-Index Resolved Length Mapping of Carbon Nanotubes in Solution Using Electric-Field Induced Differential Absorption Spectroscopy</i>
10:00-10:30	Intro Posters A: Esko Kauppinen
10:30-12:00	Coffee Break & Poster Session
12:00-12:30	Invited Talk: Jin Zhang <i>Growth of Single-Walled Carbon Nanotubes with Controlled Structure</i>
12:30-12:45	Contributed Talk: Thomas Wagberg <i>Fabrication of One Dimensional Zig-Zag [6,6]-Phenyl-C61-butyrac acid methyl ester Nanoribbons from Two Dimensional Nanosheets</i>
12:45-13:00	Contributed Talk: Hai Duong <i>Continuous and scalable fabrication and potential applications of multi-walled carbon nanotube aerogels from the floating catalyst method</i>
13:00-14:15	Lunch
14:15-14:45	Invited Talk: Jing Kong <i>High surface area, low density aerogels from one- and two-dimensional nanomaterial</i>
14:45-15:00	Contributed Talk: Hidetsugu Shiozawa <i>Molecular assembly in porous nanostructures</i>
15:00-15:15	Contributed Talk: Gerald Singer <i>CNT functionalization towards high performance composite materials</i>
15:15-15:30	Contributed Talk: Yan Li <i>Structure-controlled growth of single-walled carbon nanotubes on substrates</i>
15:30 - 16:00	Intro Posters B&C: Ralph Krupke
16:00 - 17:30	Refreshments /Posters
17:30 - ...	Walking Tour

MONDAY

KN1: Progress Towards Single Crystals of Carbon Nanotubes

Kono, Junichiro (Rice University, USA)

Despite many years of worldwide efforts, there is presently no established method for producing large-area single-domain films of highly aligned, densely packed, and chirality-enriched single-wall carbon nanotubes (SWCNTs). If developed, such a method can eventually lead to the realization of a SWCNT crystal – i.e., a 3D object consisting of a period array of SWCNTs that maintains the extraordinary properties of individual nanotubes. Here, we report a new, promising method for achieving this long-standing goal. Utilizing spontaneous alignment that occurs during vacuum filtration, we have produced a wafer-scale (i.e., inch-size) film of aligned SWCNTs [1]. This method is universal applicable to SWCNTs synthesized by different methods and can be scaled up in all three dimensions. We characterized the produced large-area films using a variety of microscopy, spectroscopy, and electronic transport techniques, demonstrating nearly perfect global alignment with a single domain. The strikingly high degree of alignment of our films with a nematic order parameter of ~ 1 and a thickness of ~ 100 nm distinguishes our method from previously reported 2D and 3D postgrowth assembly techniques. We investigated the mechanisms underlying the observed global spontaneous alignment, based on a proposed model of 2D confinement induced phase transitions. We discuss how the degree of alignment depends on the filtration speed, the SWCNT concentration, the surfactant concentration, the hydrophilicity of the filter membrane surface, the SWCNT length, and the SWCNT diameter.

[1]. X. He, W. Gao, L. Xie, B. Li, Q. Zhang, S. Lei, J. M. Robinson, E. H. Háróz, S. K. Doorn, R. Vajtai, P. M. Ajayan, W. W. Adams, R. H. Hauge, and J. Kono

CT1: Chiral-Index Resolved Length Mapping of Carbon Nanotubes in Solution Using Electric-Field Induced Differential Absorption Spectroscopy

Li, Wenshan (Karlsruhe Institute of Technology, Karlsruhe, GER); Hennrich, Frank (Karlsruhe Institute of Technology, Karlsruhe, GER); Flavel, Benjamin Scott (Karlsruhe Institute of Technology, Karlsruhe, GER); Kappes, Manfred (Karlsruhe Institute of Technology, Karlsruhe, GER); Krupke, Ralph (Karlsruhe Institute of Technology, Karlsruhe, GER)

We demonstrate a rather simple method based on electric-field induced differential absorption spectroscopy (EFIDAS) to measure the chiral-index-resolved average length of SWCNTs in dispersions [1]. The method takes advantage of the electric-field induced length-dependent dipole moment of nanotubes and has been verified and calibrated by atomic force microscopy. This method not only provides a low cost, *in-situ* approach for length measurements of SWCNTs in dispersion, but due to the sensitivity of the method to the SWCNT chiral index, the chiral-index dependent average length of fractions obtained by chromatographic sorting can also be derived. Furthermore, we report on our recent results on fabricating transistors from highly enriched semiconducting SWCNTs prepared by PODOF polymer wrapping and size-exclusion chromatography [2]. The purity of the material was determined to be > 99.7 % from the transfer characteristics of short-channel transistors comprising densely aligned sc-SWCNTs. The transistors possess a hole mobility of up to 297 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ and On/Off ratio as high as 2×10^8 .

[1] Li W, Hennrich F, Flavel S, Kappes M, Krupke R, under review.

[2] Hennrich F, Li W, Fischer R, Lebedkin S, Krupke R, Kappes M, *ACS Nano*, 10 (2016) 1888

IT1: Growth of Single-Walled Carbon Nanotubes with Controlled Structure

Zhang, Jin (Peking University, Beijing, CHN)

Direct growth single-walled carbon nanotubes (SWNTs) with controlled structures still remains many challenges. Even through many methods, aiming to optimize the interface of SWNT-catalyst or SWNT-seed for chirality-selective growth, were developed. However, the greatest difficulty impeding their moving forward to application is how to grow SWNTs with controlled structures. In this talk, we will focus on the controlled growth of SWNTs arrays with ultra-high density, high ratio semiconducting properties and special chiral angles. For the SWNTs arrays with ultra-high density, Trojan catalysts (released from substrate) was developed and the density can be as high as 150 tubes/ μm . Combining Trojan catalysts with Mo nanoparticles as cooperating catalysts, the ultra-high density SWNTs arrays with wafer-scale area can be obtained. For the SWNTs arrays with semiconducting properties, oxides catalysts with oxygen vacancy, bimetal catalysts and uniform Mo_2C catalyst were used to grow semiconducting SWNTs arrays and ratio of semiconducting tubes can be higher than 95%. For the SWNTs arrays with special chiral angles, based on the analysis the thermodynamics and kinetics of SWNTs growth, horizontally (2m, m) SWNT arrays with chiral angle of 19.1° , tubes arrays with small chiral angles (less than 10°) and near-armchair tubes ((n, n-1) or (n, n-2)) can be grown under different conditions.

[1] Growth of High-Density Horizontally Aligned SWNT Arrays using Trojan Catalysts, *Nat. Commun.* 6 (2015), 6099.

[2] Helicity-dependent single-walled carbon nanotube alignment on graphite for helical angle and handedness recognition, *Nat. Commun.* 4 (2013), 2205.

[3] Diameter-Specific Growth of Semiconducting SWNT Arrays Using Uniform Mo_2C Solid Catalyst, *J. Am. Chem. Soc.* 137(28) (2015), 8904-8907.

[4] Selective Scission of C–O and C–C Bonds in Ethanol using Bimetal Catalysts for the Preferential Growth of Semiconducting SWNT Arrays, *J. Am. Chem. Soc.* 137 (3) (2015), 1012-1015.

CT2: Fabrication of One Dimensional Zig-Zag [6,6]-Phenyl-C61-butyric acid methyl ester Nanoribbons from Two Dimensional Nanosheets

Gracia-Espino, Eduardo (Umea University, Department of Physics, Umea, SWE); Barzegar, Hamid (Department of Physics, UC Berkeley, USA, Berkeley, USA); Yan, Aiming (Department of Physics, UC Berkeley, USA, Berkeley, USA); Zettl, Alex (Department of Physics, UC Berkeley, USA, Berkeley, USA); Wagberg, Thomas (Umea University, Department of Physics, Umea, SWE)

One-dimensional (1D) zig-zag [6,6]-Phenyl-C61-butyric acid methyl ester (PCBM) nanoribbons are produced by folding two-dimensional ultrathin PCBM nanosheets in a simple solvent process. The unique 1D PCBM nanostructures exhibit uniform width of 3.8 ± 0.3 nm, equivalent to four PCBM molecules, and lengths of 20-400 nm. These nanoribbons show well-defined crystalline structure, comprising PCBM molecules in a hexagonal arrangement without trapped solvent molecules. First principle calculations and detailed experimental characterization provides an insight into the structure and formation mechanism of the 1D PCBM nanoribbons. Given their dimensions and physical properties, we foresee that these nanostructures should be ideal as acceptor material in organic solar cells.

CT3: Continuous and scalable fabrication and potential applications of multi-walled carbon nanotube aerogels from the floating catalyst method

Duong, Hai (National University of Singapore, Singapore, SGP); Tran, Thang (National University of Singapore, Singapore, SGP); Mikhalchan, Anastasiia (National University of Singapore, Singapore, SGP); Fan, Zeng (National University of Singapore, Singapore, SGP); Liu, Peng (National University of Singapore, Singapore, AUT)

We present a direct and scalable floating catalyst method to fabricate the self-supporting carbon nanotube (CNT) aerogels at higher deposition rates. The whole fabrication process takes only about 1-2 hours and can produce meter-long CNT aerogels continuously without using freeze drying and supercritical drying processes. The undeniable advantages of the established process also include its precise control of the amount of impurities and morphology of the CNT aerogel. The density of the aerogels ranges from 0.55 to 32 mg/cm³ with high porosity (>98%) and surface area of up to 170 m²/g. To the best of our knowledge, these are the first reported CNT aerogels lighter than 1 mg/cm³ and comparable with the lightest graphene aerogels ever reported. At the same time, the CNT aerogels are not brittle, easy on handling and even the lightest ones can withstand a weight of ~150 times higher than their own (~15000 times higher than its density) without collapsing. The thermal conductivity is within the range of 0.127-0.137 W/m·K. The electrical conductivity reaches up to 106 S/m, far beyond of those reported for the CNT aerogel coated with graphene, pure graphene- or graphene/CNT aerogels, and other CNT aerogels synthesized using the freeze-drying and critical point-drying methods. With different collecting techniques and after the post treatments, we can produce the super strong km-long CNT fibers having up to 5.02 GPa of tensile strength and 444 GPa of young modulus and also meter-scale aligned CNT thin films with their thermal conductivity of up to 400 W/m.K, higher than thermal conductivities of copper and aluminium.

IT2: High surface area, low density aerogels from one- and two-dimensional nanomaterial

Kong, Jing (MIT, Cambridge, USA)

Aerogels have numerous applications due to their high surface area and low densities. Creating aerogels from a large variety of materials has remained an outstanding challenge. In recent years we have developed a methodology to enable aerogel production with a wide range of materials. The method is based on the assembly of anisotropic nano-objects(1D nanotubes, nanowires or 2D nanosheets) into a cross-linking network from their colloidal suspensions at the transition from semi-dilute to isotropic concentrated regime. This method is anticipated to open up wide opportunities for the applications of aerogels in catalysis, sensing and many other energy related applications.

CT4: Molecular assembly in porous nanostructures

Shiozawa, Hidetsugu (Elektronische Materialeigenschaften, Wien, AUT); Domanov, Oleg (Faculty of Physics, University of Vienna, Vienna, AUT); Kampf Müller, Johannes (Faculty of Physics, University of Vienna, Vienna, AUT); Briones-Leon, Antonio (Faculty of Physics, University of Vienna, Vienna, AUT); Zechner, Georg (Faculty of Physics, University of Vienna, Vienna, AUT); Sato, Yuta (Nanomaterials Research Institute, AIST, Tsukuba, JPN); Suenaga, Kazu (Nanomaterials Research Institute, AIST, Tsukuba, JPN); Saito, Takeshi (Nanomaterials Research Institute, AIST, Tsukuba, AUT); Weschke, Eugen (BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, GER); Eisterer, Michael (Atomintitut, Vienna University of Technology, Vienna, AUT); Peterlik, Herwig (Faculty of Physics, University of Vienna, Vienna, AUT); Lang, Wolfgang (Faculty of Physics, University of Vienna, Vienna, AUT); Pichler, Thomas (Faculty of Physics, University of Vienna, Vienna, AUT)

Porous nanostructures, such as carbon nanotubes (CNTs) and metal-organic frameworks (MOFs), allow atoms and molecules to be assembled in 1D arrays and nanoclusters that could outperform their bulky counterparts. Our experiments using Raman, UV-Vis, photoemission, SQUID, electron microscopy and magnetotransport measurements elucidate electronic and magnetic interactions at guest-host molecular interfaces that are responsible for their unique physical properties. We show that encapsulated inside single-wall carbon nanotubes (SWCNTs) or carbon fibers, iron and nickel clusters behave as stable single-domain magnets exhibiting large coercive fields as the cluster size becomes as small as the exchange length. In MOFs, metal ions are coordinated to form metal arrays and nanovoids. Magnetic transition metal arrays in MOFs are ideal systems in which we study anisotropic magnetic coupling. Metal ions exposed to the interior voids react with infiltrating molecules, leading to MOF's sensing abilities. We show that the MOF's electrical conduction and magnetic ordering temperature can be tuned by molecular doping.

This work was supported by the Austrian Science Funds (FWF), projects P621333-N20 and P27769-N20

CT5: CNT functionalization towards high performance composite materials

Singer, Gerald (University of Natural Resources and Life Sciences Vienna, Vienna, AUT); Unterlass, Miriam M. (Technische Universität Wien, Vienna, AUT); Wendrinsky, Josef (Technische Universität Wien, Vienna, AUT); Rennhofer, Harald (University of Natural Resources and Life Sciences Vienna, Vienna, AUT); Sinn, Gerhard (University of Natural Resources and Life Sciences Vienna, Vienna, AUT); Grünewald, Tilman A. (University of Natural Resources and Life Sciences Vienna, Vienna, AUT); Windberger, Ursula (Medical University of Vienna, Vienna, AUT); Stöger, Werner (Secar Technologie GmbH, Hönigsberg, AUT); Semlitsch, Karl H. (Secar Technologie GmbH, Hönigsberg, AUT); Lichtenegger, Helga (University of Natural Resources and Life Sciences Vienna, Vienna, AUT); Unterlass, Miriam (Technische Universität Wien, Vienna, AUT); Grünewald, Tilman (University of Natural Resources and Life Sciences Vienna, Vienna, AUT); Semlitsch, Karl (Secar Technologie GmbH, Hönigsberg, AUT)

Carbon fibre reinforced composite (CFRC) materials are among the most promising new materials for high-performance applications such as lightweight construction, aeronautics or automotive industry. The high anisotropy of CFRC and outstanding mechanical properties along the fibre direction allows on the one hand for custom tailored properties for a large variety of applications but on the other hand renders the laminates susceptible to delamination normal to the fibre plane and also decreases the fatigue properties significantly. One attempt to overcome these obstacles is to add a further filler component to the composite material: Adding multi-walled carbon nanotubes (MWCNTs) can improve materials properties not only with respect to fracture properties but also higher lifetimes under cyclic loading. For the interaction of MWCNTs and the composite matrix, the dispersion and functionalization play a key role, determining the composite performance. In this work we present ongoing research on a hierarchically structured composite consisting of carbon fibre mats and epoxy (Bisphenol-A-epichlorhydrin resin with amine hardener) reinforced with functionalized MWCNTs. Homogenous dispersions were prepared by several cycles on a three-roll mill. The MWCNTs (Nanocyl NC7000) were amine-functionalized via an oxidation step followed by the reaction with a diamine. These freshly-prepared amine-functionalized MWCNTs were compared to commercially available MWCNTs with an amine-functionalization (Nanocyl NC3152). All mentioned nanotubes were studied by means of Raman-spectroscopy and XPS. For the characterization of resin and hardener GC-MS, GPC and NMR were used. Also the isomers of the amine hardener were investigated using a chiral crystallization approach. The characterizations of the epoxy system and the MWCNTs are shown together with the first results of mechanical testing.

CT6: Structure-controlled growth of single-walled carbon nanotubes on substrates

Li, Yan (Peking University, Beijing, CHN)

Single-walled carbon nanotubes (SWNTs) present structure-determined outstanding properties and SWNTs with a single (n, m) type are needed in many advanced applications. Carbon nanotubes and their caps or catalysts can all act as the structural templates to guide the formation of SWNTs with a specified chirality [1]. SWNT growth via a catalyzed chemical vapour deposition CVD process is normally more efficient and therefore of great interest. We developed a new family of catalyst, tungsten-based intermetallic nanocrystals, to grow SWNTs with specified chiral structures. Such intermetallic nanocrystals present unique structure and atomic arrangements, which are distinctly different from the normal alloy nanoparticles or simple metal nanocrystals, therefore can act as the template to grow SWNTs with designed (n, m) structures. Using W_6Co_7 catalysts, we realized the selective growth of (12, 6) [2], (16, 0) [3], (14, 4) and other chiralities. By the cooperation of thermodynamic and kinetic factors, SWNTs with high chirality purity can be obtained

[1]. The Growth of horizontally aligned SWNT arrays with specific chirality were also realized.

[1] F. Yang, X. Wang, M. Li, X. Liu, D. Zhang, J. Yang, Y. Li, *Acc. Chem. Res.*, 2016, DOI: 10.1021/acs.accounts.5b00485.

[2] F. Yang, X. Wang, D. Zhang, J. Yang, D. Luo, Z. Xu, J. Wei, J.-Q. Wang, Z. Xu, F. Peng, X. Li, R. Li, Y. Li, M. Li, X. Bai, F. Ding, Y. Li, *Nature*, 510, 522 (2014).

[3] F. Yang, X. Wang, D. Zhang, K. Qi, J. Yang, Z. Xu, M. Li, X. Zhao, X. Bai, Y. Li, *Journal of the American Chemical Society*, 137, 8688-8691 (2015)..

POSTER SESSION A: Synthesis & Processing

A1: Growth of single-walled carbon nanotube from nanotube edges with various diameters

Inoue, Taiki (The University of Tokyo, Tokyo, JPN); Takezaki, Hiroki (The University of Tokyo, Tokyo, JPN); Otsuka, Keigo (The University of Tokyo, Tokyo, JPN); Xiang, Rong (The University of Tokyo, Tokyo, JPN); Chiashi, Shohei (The University of Tokyo, Tokyo, JPN); Maruyama, Shigeo (The University of Tokyo, Tokyo, JPN)

Chirality-controlled growth of single-walled carbon nanotubes (SWCNTs) is required for the electronic application of SWCNTs. One possible strategy is to use open-end nanotubes as growth templates [1,2] instead of metal nanoparticles as catalyst. In this study, we synthesized SWCNTs from open-end nanotube templates containing various diameters and investigated the growth mechanism. Horizontally aligned SWCNTs were firstly grown from patterned iron catalyst on crystal quartz substrates. Photolithography and oxygen plasma treatment were performed to give SWCNT segments with tube edges free from metal nanoparticles. SWCNTs were grown by pretreating the nanotube segments in air and then in water vapor at various temperatures, followed by introducing ethanol as a carbon source. Raman investigation revealed that average diameter of extended SWCNTs after regrowth is smaller than that of SWCNT templates, indicating that smaller-diameter SWCNTs act as growth templates more frequently.

[1] Y. Yao et al., *Nano Lett.* 9, (2009) 1673.

[2] J. Liu et al., *Nat. Commun.* 3 (2012) 1199.

A2: A Strategy for High-Quality CVD-Grown

Shim, Gi Woong (KAIST, Daejeon, KOR) Gi Woong Shim, Sang Yoon Yang, Seung-Bum Seo, and Sung-Yool Choi () School of Electrical Engineering and Graphene Research Center, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea*

Two-dimensional (2D) materials and their van der Waals (vdW) structures have shown possibilities to enable high-performance electronics and photonics. However, quality of large-area grown samples (usually by chemical vapor deposition, CVD) is far from the requirements for the electronic materials, acting as a bottleneck for real applications. Thus, the improvement of the quality of the CVD-grown samples will be the first step to exploit the real potential of 2D materials and their van der Waals (vdW) systems. Molybdenum disulfide (MoS₂) is a representative 2D semiconducting material and the most widely investigated one among the 2D transition metal dichalcogenide family. In most cases, it is grown by a mild sulfurization of molybdenum (VI) oxides. The method for the growth has advantages in terms of simplicity, however, has many limitations in achieving uniform, scalable, and layer controllable growth, etc. To precisely control the growth, understandings on the growth system and mechanisms should be preceded, however, they are remained as unclear. As a result of the growth mostly carried out by trial-and-error, there have not been much improvements on the quality of MoS₂ up to now. Herein, we provide

novel and predictable approaches on the high-quality synthesis of MoS₂. Based on system interpretations in many perspectives, key parameters governing the growth is identified and facile strategies for improving the quality of MoS₂ are provided. Also, we identify issues and limitations for the conventional CVD growth method, and show possible route for solving such issues.

A3: Ab initio molecular dynamics study of dissociation of ethanol on nickel carbon cluster in metal-catalyzed growth of carbon nanotubes

Fukuhara, Satoru (The University of Tokyo, Tokyo, JPN); Shimojo, Fuyuki (Kumamoto University, Kumamoto, JPN); Shibuta, Yasushi (The University of Tokyo, Tokyo, JPN)

The formation mechanism of carbon nanotubes is considered to be composed of several steps i.e. dissociation of carbon source molecules, cap formation and tube growth processes. Each step has been discussed from both the experimental and computational points of view [1-3]. However, the relation between each process e.g. the effect of dissolved carbons on the dissociation process is not well understood yet. In this study, the effect of carbon in nickel cluster on the dissociation process is investigated by ab initio molecular dynamics and nudged-elastic-band (NEB) simulations to unravel the initial stage of metal-catalyzed growth process of carbon nanotubes via an alcohol catalytic chemical vapor deposition. It has been observed that ethanol molecules do not adsorb on carbon atoms in the cluster and ethanol less dissociates on nickel-carbon cluster compared to pure-nickel cluster. In addition, the NEB analysis indicates that the activation energy of the C-H bond dissociation in the fragment molecules on the nickel-carbon cluster is higher than that on the pure nickel cluster. It indicates carbon atoms in the catalyst have a negative effect on dissociation process of carbon source molecules. In the presentation, our recent results will be introduced after the brief review of recent computational works on this topic.

- [1] J.A. Elliott, Y. Shibuta, H. Amara, C. Bichara and E.C. Neyts, *Nanoscale*, 5(2013) 6662-6676.
- [2] T. Oguri, K. Shimamura, Y. Shibuta, F. Shimojo and S. Yamaguchi, *Journal of Physical Chemistry C*, 117(2013) 9983-9990.
- [3] T. Oguri, K. Shimamura, Y. Shibuta, F. Shimojo and S. Yamaguchi, *Chemical Physics Letters*, 595(2014)185-191.

A4: Aligned and continuous carbon fibers from carbon nanotube template

Liu, Peng (Tsinghua University, Beijing, CHN)

The superior mechanical, thermal, electrical and chemical properties of carbon fibers make them promising materials as electrodes of energy storage devices and carbon-fiber-reinforced plastics. To meet the demand of large-area applications, low-cost mass-production of carbon fibers should be realized. Here, we report the facile fabrication of aligned, continuous and catalyst-free carbon fibers from the carbon nanotube template. The fabrication process includes thickening of continuous carbon nanotube sheets by pyrolytic carbon deposition and graphitization of the carbon layer

by high temperature treatment. The as-fabricated carbon fibers have an annual ring structure like the tree, with carbon nanotube template at the center. The diameter of the fiber ranges from tens of nanometers to several microns, depending on the fabrication conditions. The aligned and continuous features of the fibers inherited from the parent carbon nanotube sheet together with their outstanding physical and chemical properties would certainly be meaningful to the large-area applications of carbon fibers.

A5: Chiral Angle Controlled Growth of Single-Walled Carbon Nanotubes

Zhang, Shuchen (Peking University, Beijing, CHN)

Single-walled carbon nanotubes (SWNTs) have been regarded as one of the most attractive candidates to be used as building blocks in the next generation electronics. Although many efforts were dedicated to the chirality-selective SWNT growth by using various strategies and significant advances have been reported, the randomly formed cap structure allows the nucleation of all types of SWNTs on normally liquid catalysts(Fe...etc) with high activity. Here, we develop a CVD process that allows temperature to be changed periodically to vary a SWNT's chirality frequently in order to build up a more stable catalyst-SWNT interface and the other one to obtain a stable interface through slowing down the absorption and decomposition of carbon source on catalysts. SWNTs with small helix angles(less than 10°), which are predicted to have lower interfacial formation energy than others. While a zigzag tube is hard to grow during the normal CVD process, kinetic analysis of the process suggests a multiple redistribution features that a large chiral angle SWNT tends to reach the near zigzag chirality step by step with a small chiral angle change every step, named as "Tandem-Plate CVD". And the tubes with small chiral angles are enriched up to 72%. On the other hand, when slowing down the absorption and decomposition of carbon source on liquid catalysts to meet the thermodynamics-stable catalyst-SWNT interface, no zigzag tubes appeared and on the contrary, near-armchair tubes, (n, n-1) or (n, n-2), with large helix angles would be enriched, who are semiconducting. These methods open a new door to enrich those SWNTs with more stable catalyst-tube interfaces experimentally.

A6: Chirality selective synthesis of single-walled carbon nanotubes with sputtered W-based catalyst

An, Hua (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN); Xiang, Rong; Takezaki, Hiroki; Ohyama, Shinnosuke; Qian, Yang; Inoue, Taiki; Chiashi, Shohei; Maruyama, Shigeo

Single-walled carbon nanotubes (SWNTs) have been regarded as one of the most promising building-blocks in nanoelectronics due to their chirality-dependent properties. However, the potential industrial applications are impeded by the mixed chiralities of as-grown SWNT assemblies. Direct synthesis of SWNTs with single chirality is challenging but attracts considerable attention among researchers. Catalyst plays an important role in the chirality controlled synthesis of SWNTs.

Recently, Co₇W₆ clusters were reported to successfully grow a single chirality SWNT (12, 6), with over 90% abundance and a zigzag SWNT (16, 0), with near 80%, by controlling the catalyst structure and growth conditions with a high-temperature reduction and growth [1, 2].

In this report, we show that the sputtered CoW catalyst can selectively grow (12, 6) SWNTs with better uniformity by low pressure chemical vapor deposition at lower temperature [3]. The abundance of (12, 6) is over 50% according to the statistical Raman mapping analysis and optical absorption spectrum of the as-grown SWNTs. Parametric study of the CoW catalyst system demonstrates that the reduction temperature before growth is critical for the selectivity and the intermediate structure, Co₆W₆C, is identified by the electron diffraction. Moreover, the investigation of catalysts discloses the complicated structure changes before and after growth. Time-dependent selectivity and the structure evolution of catalysts will be discussed in detail.

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[2] F. Yang et al., *J. Am. Chem. Soc.* 137, 8688 (2015).

[3] S. Maruyama et al., *Chem. Phys. Lett.* 360, 229 (2002).

A7: Confined linear carbon chains: Synthesis and properties

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The extreme instability and strong chemical activity of carbyne, the infinite sp¹ hybridized carbon chain, are responsible for its low possibility to survive at ambient conditions. We successfully synthesized extremely long linear carbon chains (LLCCs) inside thin double walled carbon nanotubes as nanoreactors and protectors [1]. Their existence, structure, lengths and yield have been proved by Raman, HRTEM, STEM and XRD. The results show that the single-triple bonded LLCCs including thousands of carbon atoms have at least six new Raman peaks, some of which are even stronger than the G-band. The optimum growth conditions, for example, diameter of the host tubes, annealing temperatures and time were carefully studied. The interaction and charge transfer between the LLCCs and their host nanotubes were explored using resonance Raman, low-temperature Raman and DFT calculations [2]. Furthermore, the band gap of the LLCCs was examined by resonance Raman spectroscopy. The

results suggest that the band gap of LLCCs in the range of 1.8 - 2.3 eV is inversely proportional to their lengths, which is also perfectly consistent with our DFT calculations [3].

L. S., T.P. thank the FWF, P.A. acknowledges the EU.

[1] Shi et al. Nature Materials doi:10.1038/nmat4617

[2] Wanko et al. arXiv:1604.00483

[3] Shi et al. Band gap of long linear carbon chains. In preparation.

A8: Controllable Synthesis of MgO-templated Carbon Nanostructures via Simple Carbonization Confined linear carbon chains: Synthesis and properties

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Recently, mesoporous carbons have wide applications from private houses to industrial factories. It can be used as adsorbents for removal of hazards and toxic materials like organic dyes or heavy metals and also can be used as electrode materials for energy storage devices. Templated-carbonization process represents a simple way to produce nanocarbon exhibiting porous feature. MgO is one of the suitable, easy and simple templates for the production of porous nanocarbon. It can be easily dissolved in diluted acid. The pore structure of produced nanocarbon is usually homogeneous. Moreover, this process is able to use thermoplastic precursors as carbon sources. In this regard, mesoporous MgO template was synthesized via simple co-precipitation method from magnesium hydride precursor. The carbonization process was carried out to yield mesoporous carbon from MgO template impregnated with polyacrylic acid or sucrose into it as carbon sources. The effect of carbonization temperature and carbon sources was also studied. The produced structures were investigated with the help of XRD, TEM, FTIR and Raman spectroscopy. The results showed the formation of graphitic nanostructures. We expect that this simple carbonization has high possibility to apply for production of mesoporous carbon in a large scale.

A9: Controlled growth of nanosheet-carbon nanotube heterostructures

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Nanomaterials have drawn continuous attention by virtue of their versatile structures and unique properties. It is believed that controlled synthesis of three-dimensional nanostructures, constructed with fundamental nanoscale building blocks, have great potential to integrate their merits and explore exotic phenomena. Among these, it is hard to epitaxially grow two-dimensional (2D) nanostructures on one-dimensional (1D) nanomaterials, since it is expected to completely expose the lateral nano-edge of

2D materials. Here, we present a strategy to synthesize hexagonal and quadrangular nanosheets of molybdenum compound on individual ultralong carbon nanotubes (CNTs), where the as-grown CNTs lying on a substrate acted as backbones and nanosheets were selectively deposited on the CNTs and grown out of the plane of the substrate. These nanosheet-CNT heterostructures, which may possess unique electronic and optical properties, are believed to have great potentials in development of novel devices.

A10: Correlation of catalyst surface states and chirality distribution of single-walled carbon nanotubes during plasma CVD Controlled growth of nanosheet-carbon nanotube heterostructures

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Single-walled carbon nanotubes (SWNTs) have many outstanding properties due to the unique one dimension tubular structures. Since the physical properties of SWNTs is strongly influenced by the chirality, chirality - controlled synthesis of SWNTs is still regarded as an ultimate subject in this scientific community. Our group has realized the narrow chirality-distributed growth of SWNTs with the precisely - controlled plasma CVD [1-3]. However, elucidation of the correlation of catalyst structures and surface states with the chirality species remains as an important issue towards perfect chirality-controlled synthesis of SWNTs. Based on this background, systematical investigations were carried out aiming for the elucidation of the correlation between catalyst states and chirality distributions. The catalyst structures and surface state were analyzed by atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM). We find out that the dominant chirality species in the narrow chirality-distributed SWNTs is very sensitive to the surface state of catalyst, which can be tuned by the appropriate surface treatments. We believe that our findings can contribute to the growth of chirality-controlled SWNTs.

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[3] B. Xu, T. Kato, K. Murakoshi, and T. Kaneko, J. Plasma Fusion Res. **9**, 1206075 (2014).

A11: Development of Gel Chromatography Method for High Yield Metal/Semiconductor Separation of Carbon Nanotubes

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Single walled carbon nanotubes (SWCNTs) have extraordinary electrical, optical, mechanical and thermal features that draw attention in numerous fields. However, SWCNTs are generally fabricated as mixtures (one third of metallic and two thirds of semiconducting) containing many different diameter ranges and chiral species. In this aspect, separation of different types of SWCNTs are fundamental for usage of potential application. For instance, in solar cells, semiconducting SWCNTs are

extremely required in active layer. In thin films, diameter selectivity is also significant due to the fact that small diameter SWCNTs raise open circuit voltage (Voc) and improve charge separation while large diameter SWCNTs provide to gain large mobility by decreasing contact resistance. In this purpose, gel chromatography is one of the most used technique for separation of SWCNTs because of low cost, simple and large scale. Here, we reported for the first time that instead of bulk SWCNT solution (bottom phase after the first column), metallic and unbound SWCNT mixture (after 1% SDS) was iteratively flowed through repeated columns using binary desorption system. In this way, we achieved to obtain highly enriched metallic and small diameter semiconducting SWCNTs with nearly single chirality. The separation achieved was verified by UV-vis -NIR and Raman spectroscopy.

[1] Wang, H. et al. ACS Nano 2014, 8, 2609–2617

[2] Liu, H. et al. Nat. Commun. 2011, 1-8

A12: Effect of different bilayer catalyst configurations on quality and electronic type selectivity of CVD grown SWCNTs

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Wafer-level synthesis of semiconducting SWCNTs (s-SWCNTs) with high degree of purity and quality are crucial prerequisites for industrial realization of electronic devices with SWCNT-based transistors and sensors. Catalytic chemical vapor deposition (CCVD) is considered as a promising approach for SWCNT integration in particular from the vantage point of scalability and controllability [1]. However, wafer level CVD grown s-SWCNTs are not yet pure and selective enough for direct use in devices. Here we present the progress on a wafer level compatible technique for reliable and reproducible catalyst deposition followed by CVD growth of SWCNTs. We have focused our investigations on different bilayer catalyst configurations such as Co-Mo, Co-Ni, Ni-Mo and Co-Ru. With a special in-situ sample preparation procedure, a set of different catalyst thicknesses for each bilayer catalyst configuration were prepared by ion beam sputter deposition on each wafer substrate. Those wafers were exposed to CVD processes in a vertical CVD reactor. A comparative study correlating different catalyst configurations and properties of corresponding CVD-grown SWCNTs was conducted by means of Raman spectroscopy and SEM analysis. Results indicate in case of bilayer catalyst systems, electronic type-selectivity as well as quality of grown SWCNTs are strongly determined by the right thicknesses of bilayer catalysts components. We demonstrate that our special procedure allows a fast localization of optimized process conditions for type-enriched SWCNTs coatings especially for wafer-level processes with multi-catalyst systems.

[1] E. Aasmundtveit et al., Material 6, 2013

A13: Efficient CVD growth of super-small diameter single-walled carbon nanotubes

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Super-small diameter single-walled carbon nanotubes (SWNTs) smaller than (6,5) (~0.8 nm) are known to be very inefficient to grow and observe unless inside of special zeolite pore or inside of an outer nanotube. Here we report the efficient growth results for super-small diameter SWNTs by extending the work window of conventional chemical vapor deposition (CVD). CVD temperature was varied from 350 oC to 900 oC combined with the pressures range over 5 magnitudes. Resonant Raman with 5 excitation laser lines, absorption and photoluminescence (PL) were used to characterize the chirality and abundance of SWNTs. Super-small diameter SWNTs assigned as (6,4), (5,4), (5,3), (6,1) etc.. (0.8 nm > dt > 0.52 nm) were obtained around 500 oC, 5 Pa, and their abundances were significantly increased comparing to previous reported works. In addition, growth mechanism is clarified through kinetic discussion on the experimental map of extended CVD. The relationship of temperature and pressure was identified: SWNTs can grow in lower CVD temperature accompanied with proper lower pressure.

A14: Efficient synthesis of millimeter-tall SWNT forests on a MgO catalyst support enabled by a simple pretreatment process

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When single-wall carbon nanotubes (SWNTs) are efficiently grown from a substrate by chemical vapor deposition, they assemble in a vertically aligned array of SWNTs, which are long and of high purity (forest). To achieve high efficiency, aluminum oxide (Al₂O₃) layer has been recognized to play an important role to support the formation of dense and small iron catalyst particles [1]. In contrast, millimeter-scale SWNT forests have rarely been reported using catalyst supports not containing Al, and the fundamental reason for this difficulty is not yet well understood. Magnesium oxide (MgO) is one of the alternative materials commonly used for catalyst support [2]; however, the growth efficiency of SWNT forest has been quite low compared with using Al₂O₃.

In this study, we have examined the preparation method of MgO support, and successfully demonstrated the efficient synthesis of SWNT forests exceeding 1 mm height with a catalyst support other than Al₂O₃. Annealing (750°C in air) the sputtered MgO film was found to be a critical process to obtain catalyst support suitable for the synthesis of tall forests. By using the water-assisted CVD method (in 10 min) [3], forest heights exceeded 1.2 mm, which was comparable to that obtained by using Al₂O₃ support layers. In-situ height measurement revealed that the lifetime of the forest growth was similar to that observed for Al₂O₃ with a lifetime exceeding 10 minutes. Transmission electron microscopy revealed that most of the CNTs (>90%) were SWNTs. Since MgO is inexpensive and commonly used material, our results present an additional route in the economical and scalable catalyst preparation process for SWNT mass production. This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

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A15: Etching Behavior of Carbon Nanotubes

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Gas phase etching plays an important role in the selective enrichment of single-walled carbon nanotube (SWNT) with specific structures, which is of great importance in its future applications, and shows dramatic performance. Various etching agents, including O₂, H₂O, CO₂, etc, had been reported to have selectivities in etching metallic and small diameter carbon nanotubes. During recent years, a series of ex-situ characterizations and in-situ Raman spectroscopy have been used to reveal the etching process. However, ex-situ methods could not provide real-time information of the growth process, while in-situ Raman spectroscopy could not give straightforward image of SWNTs during etching. As a result, the kinetic picture of this process was still unsharp. To overcome this gap, a highly environment-tolerant and real-time imaging method is urgently required. In this work, polarized optical microscopy [1] was used to supervise the etching process of carbon nanotubes. With this method, we found an uncontinuous and self-terminating etching model. Based on the newly observed model, the dependency between etching rates and carbon nanotube structures had also been studied. Unexpectedly, our results show that the etching rate was irrelevant to the structure of an SWNT, including its diameter, chiral angle and electronic properties. This abnormal phenomenon indicates that the adsorbates, such as surfactants and residual PMMA could significantly accelerate the etching process, and the selective adsorption should be the source of the selective etching of carbon nanotubes. This discovery contributed to the deeper understanding of the etching process of low-dimensional carbon materials, and could provide positive guidance in gas phase etching area of SWNTs.

[1] Kaihui Liu, et al. , *Nat. Nanotech.* , 2013 , 8, 917 .

A16: Fabrication of carbon nanotube embedded structure in ZnO

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Carbon nanotubes (CNTs) can be applied in optical devices, because of their considerably unique optical properties. The mode locker has been demonstrated in free-space optics and fiber-based optics, which realized a narrow pulse width mode-locked laser. So far, studies on fabrication of optical devices using CNT have been conducted, in which the CNT is embedded in organic polymer. However, the organic polymer can be degraded depending on the temperature, humidity, and intensity of the incident light. To overcome this problem, we tried to embed CNTs in an inorganic material, especially ZnO. The ZnO films were formed using the chemical solution deposition technique. The precursor solutions of ZnO were dropped on an Si or SiO₂ substrate and spin-coated at 500 rpm for 40 s. The CNT-dispersed solution was added in this process at different concentrations. The films were then rapidly heated using a ramp annealing system under vacuum for 1 h. As a result, the ZnO films, including CNTs, were obtained. To evaluate the structural properties, atomic force microscopy and scanning electron microscopy (SEM) were used. The existence of CNTs in the ZnO film was clearly confirmed by SEM of the cross-sections of the sample. In Raman spectroscopy, D- and G-band signals were observed. Therefore, the CNT structure was not destroyed in the ZnO baking process. In addition, it was found that the sample absorbs light in the 1550-nm wavelength region, as shown in Fourier transform infrared spectroscopy. These results show that the CNTs embedded in ZnO can be used to develop optical devices for fiber-optic communications systems.

A17: Facile synthesis of graphene quantum dots by microplasma-assisted electrochemistry

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In recent years, Graphene-based materials have attracted much attention due to their superior physical and chemical characteristics. However, these characteristics depend on their size and structure. Among these materials are zero-dimensional Graphene quantum dots (GQDs) with sizes defined lower than 100 nm. The electrons could be confined by the structure and let material possess semiconductor characteristic. They are also non-toxic and biocompatible making them widely applicable in biosensing, biomaging. Currently, most methods of synthesis GQD involve high temperature, costly and complex processes unfavorable to its development. Here we report a facile and rapid process to synthesize GQD through a microplasma-assisted electrochemistry method. Microplasmas are defined as gaseous discharges formed in electrode geometries where at least one dimension is less than 1mm. It can be operated with an aqueous solution as an electrode. Energetic species including

radicals, ions and electrons formed in the microplasma are capable of initiating electrochemical or non-electrochemical reactions below the electrolyte and produce GQD. Detailed materials characterizations including UV-Vis, Raman, and photoluminescence spectroscopies, and microscopies including TEM and AFM suggest the developed microplasma-assisted electrochemistry method possess the ability to produce GQDs. The analytic results demonstrate the as-product had blue emission under 365 nm UV-light. Raman spectrum show G, D and 2D band signals typical for carbon containing materials. Size distribution from TEM imaging show an average size of 4.9 nm. Finally, the PL spectrum show the emission property of as-product is excitation-dependent. Further functional group analysis will done by such as XPS and FTIR.

A18: Flexible, Strong and High Thermal Conductivity Carbon Nanotube/Graphene Films

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Rapidly manufacturing flexible and wearable electronic devices require thermal management materials which have high thermal conductivity and structural flexibility with mechanical robustness.^[1-2] However, most thermal management materials now are relatively rigid. We reported a hybrid films that were fabricated by in-situ coating of graphene oxide (GO) sheets onto the aligned carbon nanotubes (CNTs) during the film winding. It was found that high-temperature annealing could dramatically increase the film's thermal conductivity as high as 1500W/mK, and the mechanical strength up to 1GPa with extraordinary structural flexibility. The effects of the GO content, annealing temperature, as well as the measuring temperature have been systematically investigated. Meanwhile, both experimental characterizations and atomistic simulations have been implemented to study the structure evolution and the synergistic effect between CNTs and graphenes of the hybrid film under high temperature thermal annealing. The high thermal conductivity hybrid nanocarbon films with strong mechanical performance demonstrate potential applications in flexible and wearable electronics.

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[2] Miao Wang, et al. *J. Am. Chem. Soc.* , **2014** , 136: 18156.

A19: Fluidized-bed production of submillimeter-long single-wall carbon nanotubes using C₂H₄ and CO₂ feed gas

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Mass production of carbon nanotubes (CNTs) is highly demanded for their wide use in practical applications. Fluidized-bed chemical vapor deposition (FBCVD) has been emerged as a practical method to synthesize CNTs because of its high productivity [1].

Porous catalyst supports enable high productivity but cause CNTs agglomerated with them. We previously reported submillimeter-long CNTs by FBCVD using ceramic beads with flat surfaces; few-wall CNTs semi-continuously [2,3] and single-wall CNTs (SWCNTs) in batch [4]. Highly reactive C_2H_2 was fed with H_2O vapor at low concentration and high flow rate. Such gas condition realized efficient conversion of C_2H_2 at a carbon yield of 70% in a residence time of ~ 0.3 s, however, wasted a large amount of carrier gas. Here, we report FBCVD synthesis of SWCNTs using less reactive C_2H_4 and CO_2 at higher concentrations in place of C_2H_2 and H_2O vapor. Fe (1 nm)/Al (15 nm) catalyst is deposited on Al_2O_3 beads with a 0.3 mm diameter by sputtering. The catalyst is annealed by flowing 10 % H_2/N_2 at 850 °C for 5 min, and then CNTs were synthesized by FBCVD at the conditions of 20 % C_2H_4 /10 % $H_2/0-10$ % CO_2/N_2 , at 850 °C for 10 min. We have synthesized sub-millimeter long SWCNTs with a diameter of 2.6 nm at the highest carbon yield of 20%. We also show that CO_2 concentration in the reactor is a key parameter to determine the length and yield of SWCNTs.

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[3] Z. Chen, et al., Carbon 80, 1972 (2014).

[4] D.Y. Kim, et al., Carbon 50, 1538 (2012).

A20: Graphene Encapsulated Copper Nanoparticles

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The significance of printed electronics has been growing with the increasing interest in flexible device. Printed electronics gives the possibility to pattern electronic circuits simultaneously without going through a series of steps. The important and most critical element for the application of printed electronics is the conductive ink. The conductive inks are mostly based on Ag or Au nanoparticles, due to their low conductivity and high stability. However, because of their high cost, Cu is the most evident candidate to substitute. Cu is inexpensive and has good electrical and thermal properties, but it is easily oxidized in air. A promising solution is to use graphene as a protective coating on the Cu nanoparticle. Graphene has a higher electrical current density and higher thermal mobility than copper, and it is chemically stable. The poster represent our process and results of encapsulation Cu nanoparticles by graphene. Cu nanoparticles solutions were spin coated on Si/SiO₂ wafers. The graphene's growth processes were done in our CVD system, in Ar+H₂ atmosphere, at different temperatures. We developed a new method for graphene encapsulation of Cu nanoparticles. The analysis shows Cu nanoparticles encapsulated by approximately 3-4 graphene layers, without Cu oxide and without polymer residue.

A21: Growth of Horizontal Semiconducting SWNT Arrays with High Density using Ethanol/Methane CVD

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Horizontally aligned high-density and semiconducting single-walled carbon nanotube (s-SWNT) arrays are highly desirable for future electronic devices due to their superior electrical properties.^[1] However, simultaneously obtaining s-SWNT arrays with high purity and high density is extremely challenging. Recently, our group developed a new designed catalyst called Trojan or Trojan-Mo catalyst.^[2-3] It's an effective approach for growing SWNT arrays with high density over 130 tubes/ μm on sapphire surface. On the base of Trojan-Mo catalysts, we reported herein a rational method, ethanol/methane chemical vapor deposition (CVD), to grow SWNTs array with the s-SWNTs ratio over 91% and with the density as high as 100 tubes/ μm . In this method, under certain temperature, ethanol was fully thermal decomposed to feed carbon atoms for Trojan-Mo catalysts growing high density SWNT arrays. While the incomplete pyrolysis of methane provided appropriate active H radicals with the help of catalytic sapphire surface to inhibit metallic SWNTs (m-SWNTs) growth. The synergistic effect in ethanol/methane mixtures resulted in semiconducting SWNTs enriched and no obvious decrease in nanotube density due to their milder reactivity and higher controllability at suitable growth condition. This work represents a step forward in large-area synthesis of high density s-SWNT arrays on substrates and demonstrates potential applications in scalable carbon nanotube electronics.

[1] Franklin, A. D. *Nature*, **2013**, 498 : 443.

[2] Yue Hu, et al. *Nature Commun.*, **2015**, 6 : 6099.

[3] Lixing Kang, et al. *Nano Res.*, **2015**, 8 : 3694.

A22: Growth of Horizontally Aligned Chirality-Specific Single-Walled Carbon Nanotubes

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The controlled growth of chemically pristine SWNT samples with well-aligned arrays of pure chirality is a crucial issue for the high-performance and integrated circuits and has been a great challenge for two decades [1]. Recently, tungsten-based intermetallic catalyst with the desired atomic arrangements in their crystal planes can act as structural templates for chirality-specific growth of SWNTs [2-4]. We have developed herein an approach for the growth of horizontally aligned chirality-specific

SWNTs using uniform W6Co7 nanoparticles as catalysts on the sapphire surface. Using the uniform W6Co7 nanoparticles as structural templated catalysts, we are able to grow the high abundance of the (14,4) and (18,7) SWNT arrays on the sapphire surface at the optimized growth condition, respectively. Our findings open up the possibility of the wafer-scale growth of aligned chirality-specific SWNTs by using uniform intermetallic nanoparticles as catalysts for practical nanoelectronics applications. Corresponding Author: Yan Li E-mail: yanli@pku.edu.cn

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[2] F. Yang, Y. Li et al. Nature 510, 522 (2014).

[3] F. Yang, Y. Li et al. J. Am. Chem. Soc. 137, 8688 (2015).

[4] F. Yang, Y. Li et al. Acc. Chem. Res. in press (2016).

A23: Growth Of SWNTs from controlled bi-metallic Catalyst nanoparticles

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Single wall carbon nanotubes are seen as excellent candidate for application in nanoelectronic devices because of their remarkable electronic and mechanical properties [1]. These unique properties are highly dependent on their chiral structures and diameter [2]. Therefore, structure controlled growth of SWNTs, especially directly on final device's substrate, are highly desired for the fabrication of SWNT-based electronics. In this work, we present a new approach to control the diameter of SWNTs and eventually their chirality. Because of their potential to control the SWNT's chirality [3], bi-metallic nanoparticles are used to prepare alloy nanoclusters with specific structure. The catalyst nanoparticles are pre-formed following a previously described process [4]. Briefly, the oxide surface is first covered with a SAM (self-assembled monolayer) of a pyridine-functionalized silane. Then, bi-metallic (Fe-Ru, Co-Ru and Ni-Ru) complexes are assembled by coordination bonds on the pre-formed organic SAM. The resultant alloy nanoclusters are then used to catalyze SWNTs growth on SiO₂/Si substrates via CH₄/H₂ double hot-filament chemical vapor deposition (d-HFCVD). The microscopy (TEM, SEM) and spectroscopy (Raman) analysis demonstrate the high quality of SWNTs. By changing CVD temperature from 700 to 1000°C we succeeded to modulated the percentage of semi-conductor tube from 47 % to 85 %, according to Raman spectroscopy. The nanotubes were furthermore integrated into high-quality SWNT-FET with on/off ratio reaching up to seven decades.

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A24: Growth Of 3-D Carbon Nanostructures Full Of Defects On Cobalt - Copper Substrates By Chemical Vapor Deposition

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The recent advances on the synthesis methods of carbon nanotubes (CNT) have improved the quality and yield of sample production. It is well known that parameters such as metal catalyst, substrate materials, precursors or growth temperature play a crucial role in the growth of the MWCNT [1-2]. Nowadays, with sophisticated CVD experiments it is possible to synthesize different carbon nanostructures such as nanoribbons, nanohorns, nano onions, nitrogen doped (N-MWCNT), among others [3]. In this work, nitrogen doped three-dimensional networks of carbon nanotubes were produced by chemical vapor deposition (CVD) on cobalt/copper thin film. The CVD experimental setup consisted of two tubular furnaces arranged one after another (first furnace is heated up to 750 °C and the second up to 850 °C) using benzylamine, thiophene and ethanol as a carbon, nitrogen and sulfur sources. Transmission electron microscopy (TEM), scanning electron microscopy (SEM), Raman spectroscopy and X-ray diffraction characterizations were performed. Our characterizations revealed that the samples exhibit interesting features. The cobalt-copper nanoparticles weave elongated carbon nanostructure with a complicated morphology, it was observed a strong competition between carbon nanotubes and wrinkled paper-like material growth. This new material with several defects and with a large superficial area could be used in diverse biological and environmental applications

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A25: High Quality GaN Epitaxial Layers Grown on CNT-Patterned Sapphire Substrates

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Semiconductor lighting is attracting extensive attention, because of its effective reduction of lighting-induced carbon dioxide emission whilst being mercury-free. Having been commercialized into blue and green light-emitting diodes (LEDs) for years, gallium nitride (GaN) system materials are usually heteroepitaxially grown on a sapphire substrate. However, the lattice and thermal mismatch between sapphire and GaN dramatically deteriorated the quality of material and device performance on it. The patterned sapphire substrates (PSS) and lateral overgrowth techniques are successful solutions. However, the patterning processes are complicated, costly and not environmentally friendly. Here we developed a CNT-patterned sapphire substrate (CPSS) by coating sapphire substrates with super-aligned CNT films.^[1-5] High quality

GaN was grown on CPSS by metal-organic vapor phase epitaxy system. Performance of LED manufactured on CPSS was also clearly improved. This efficient, mass producible and environmentally friendly technology holds promise for industrialization.

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A26: Hydrocarbon based Floating Catalyst CVD synthesis of SWCNTs using Nitrogen as carrier gas

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The single-walled carbon nanotubes (SWCNT) thin film stands as a strong candidate for replacement of indium-tin oxide (ITO) in transparent electrodes. The length of nanotubes is critical to achieve high conductivity SWCNTs transparent conducting films (TCF) due to smaller number of resistive junctions with the longer tubes (1). The synthesis process of using carbon monoxide (CO) as carbon source is limited to produce longer SWCNTs owing to its thermodynamically limited i.e. rather low synthesis temperature. Moreover, the CO process has usually low yield, and CO is expensive and challenging to operate safely. In this contribution, we demonstrate high yield synthesis of SWCNTs in floating catalyst CVD (FC-CVD) using C₂H₄ hydrocarbon as the carbon source and nitrogen with small amount of hydrogen as the carrier gas. The nitrogen environment makes the SWCNTs growth process operation safer and also largely cuts the running cost. Our results show that the C₂H₄-N₂-H₂ FC-CVD reactor operated at 1050 °C and using ferrocene vapor based Fe catalyst particles produced relatively long bundles with an average length up to 16 μm, while the similar reactor operated at CO produced tubes with just 4 μm average length. This ethylene process produced long SWCNTs while keeping mean diameter below 1.5 nm. With such long SWCNTs, highly conductive transparent films were achieved, with the sheet resistance of 200 ohm/sq. at 90 % transmittance at a wavelength of 550nm without doping. The doping the film with gold chloride (AuCl₃) in acetonitrile solution further reduced the sheet resistance down to 60 ohm/sq. at 90% transmittance at 550 nm.

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A27: In Situ Study Of The Activation Bimetallic Catalyst For Multi-walled Carbon Nanotubes Growth

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Despite significant efforts, the CCVD synthesis of multi-walled carbon nanotubes with tailored characteristics is still challenging. Catalyst nature and reaction conditions embedded in multi-step mechanism create a complex puzzle of experimental data. Using in situ XRD and in situ XPS, we separately studied the reduction of active metal species, their sintering, and carbon dissolution in catalyst. We found that the rate of the sintering of active particles determines the diameter of forthcoming nanotube. Due to the segregation, carbon species tend to concentrate on the surface or at subsurface layers of metallic species, that leads to insignificant carbon content in the core of small catalyst particles (<50 nm). Using Raman spectroscopy, we studied a ratio of intensities of 2D (two-phonon scattering) and D (disorder-induced) bands (I_{2D}/I_D) as a function of catalyst composition, size, synthesis conditions. Each type of catalyst provides the linear dependence with its own specific slope. The difference in slope can be explained in terms of differences in kinetics and energy parameters of the main steps of MWCNT growth for different type catalysts. We consider the graphene fragments to form a mosaic grain-boundary structure of nanotube walls [S.N. Bokova-Sirosh et al. / Journal of Nanophotonics, 2016), 012526]. The data obtained can be used to provide the process kinetic model development and to optimize the synthesis conditions to produce MWCNT with controlled properties.

A28: In-Plane TEM Imaging of Catalyst for SWNT Growth at High Temperature

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Catalyst is critical for the formation of single walled carbon nanotubes (SWNTs), while obtaining the intrinsic morphology and structure of these nano-sized particles at growth or near-growth conditions remains challenging. We propose an in-plane TEM approach, which enables a direct characterization of catalyst particles with atomic resolutions on a MEMS-fabricated thin SiO₂ film. Advantages of this protocol over conventional methods are: 1) catalyst are prepared and SWNTs are grown

directly on SiO₂ film so that intrinsic morphology is maintained; 2) collective (rather than localized) information from many particles can be obtained simultaneously by in-plane imaging or electron diffraction; 3) samples can be heated inside TEM and thereby catalyst behavior at high temperatures can be studied. With this new technique, we systematically investigated mono-metallic particles including Co, Fe, Ni, Pd, Pt, W, and bi-metallic catalyst including Co-Mo, Fe-Al, Co-Cu and Co-W. For example, we demonstrate that, with addition of Cu, much smaller Co particles form epitaxially on Cu and produce all sub-nm vertically aligned SWNTs. [1] In Co-W, we clearly identify an intermediate Co₆W₆C structure that is capable of producing SWNTs with a (12,6) chirality enrichment up to 70%. [2] We believe this in-plane TEM technique provides atomic yet statistic information that is so far the closest to a realistic growth process.

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A29: Large scale of synthesis of whisker carbon nanotubes

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Abstract: A new type of carbon nanotube(CNT) was synthesized. The carbon nanotubes with line structure feature named as whisker carbon nanotube (WhiskerCNT). WhiskerCNT was synthesized by catalytic chemical vapor deposition (CVD) at a growth temperature of around 1200 °C . Toluene was used as carbon feedstock, organic-metallic compound (ferrocene) as a catalyst precursor, thiophene as growth promotion agent and hydrogen as carrier gas. The productivity of the WhiskerCNT s is about 1 kg/h . T he following thermal treatment of WhiskerCNT s was carried out at 2800 °C . The morphology of the WhiskerCNT s seem different from traditional CNTs . The WhiskerCNT s be have line structure and looks like “ toothpick or whisker ” . After high temperature treatment, high graphitization of WhiskerCNT s were obtained with a crystallinity of over 95% . The WhiskerCNTs have diameters ranging from 60 to 150 nm. The WhiskerCNT s can be easily dispersed in matrix comparing with traditional CNTs which are entwined together. Raman spectra show the I G /I D ratios reached 4.16 which means that a high crystallinity and XRD also shows that the crystallinity of WhiskerCNTs reached over 95 % . The WhiskerCNT s have large aspect ratios (50m² /g) and volume density (0.005g/cm³) . The im purity of whisker carbon nanotube s is below 50 ppm. T hese unusual carbon nanotubes as a functional filler in lithium ion battery, lithium-sulphur battery and various composites will be realized due to our large-scale

production and their stabilized properties , high purity and high crystallinity
Keywords: Carbon nanotubes; whisker carbon nanotubes ; CVD ; graphitization ;

A30: Large-scale Synthesis of Multi-walled Carbon Nanotubes Using Floating Copper Catalysts

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Structure-uncontrollable processes, low-synthetic efficiency and undesired by-products (e.g. amorphous carbon) are three main factors limit CNT developments and further real-life applications. Catalytic chemical vapour deposition (CCVD) is a promising route to solve the above mentioned problems and has been demonstrated with new concepts in several reports. Herein, we aim to achieve the CNT growth with a large-scale production by controlling the carbon-diffusion pathway through the floating copper catalysts. Actually, the floating copper catalysts was regarded inert for the CNT growth. Here, we precisely controlled the flowing way of the carbon feedstock as well as the formation of copper nanoparticles and found the floating method can generate high yield comparing with conventional copper-based catalysts. This CNT growth using floating copper catalysts will give new insights for CNT growth through non-magnetic metal nanoparticles.

A31: Liquid Crystalline Phase of Functionalized Single-Walled Carbon Nanotubes in Chlorosulfonic Acid

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One of the most important issues for using single walled carbon nanotubes (SWCNTs) in a range of applications is dispersing SWCNTs in desired solvent. To date, there have been intense researches to make homogeneous dispersions of SWCNTs with no additives, but chlorosulfonic acid (CSA) is known as the only thermodynamic solvent of SWCNTs. Based on CSA dispersion, SWCNTs can be solely dissolved and highly concentrated enough to induce lyotropic liquid crystalline (LC) phase. It is known that high crystalline SWCNTs having G/D ratio over 10 is prerequisite for dissolving in CSA, indicating that functionalization of SWCNTs does not meet with criteria of LC phase of SWCNTs. In this study, we introduce LC phase of functionalized SWCNTs. The SWCNTs produced by floating catalyst chemical vapor deposition was functionalized by oxidizing in acid treatments, resulting in carboxyl group on SWCNTs surface. In addition, the amination was carried out by conjugation of ethylene diamine via EDC coupling reaction. Upon increasing mass of both functionalized SWCNTs in CSA under crossed polarizer, each sample shows schlieren texture, typical nematic texture of liquid crystalline phase. Moreover, our functionalized SWCNTs shows real spontaneous dissolution in CSA without any stirring or shaking.

A32: Macroassemblies from carbon nanomaterials of highly-defined structure

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Carbon nanomaterials such as graphene and carbon nanotubes (CNTs) have shown great promise for electrical, thermal and mechanical applications. Individual nanotubes or graphene flakes are able to outperform common materials by orders of magnitude in terms of e.g. current carrying capacity and thermal conductivity. The main problem however is in translating these properties from nanoscale into macroscale. As a consequence, the performance of macroassemblies from carbon nanostructures is still far from the limits of these materials. In addition to the problem of junctions present between individual nanotubes and graphene flakes, one of the most significant underlying reasons for that is in the lack of control over the material composition. Macrostructures from carbon nanomaterials such as fibers or films are composed from largely indiscriminate mixture of nanocarbon what has a deleterious effect on the material properties. It has not been practically possible to produce materials of purely metallic/semi-conductive character or particular chirality at the reasonable scale and thus we could not fully exploit their properties. We have developed a process which can produce highly-defined macrostructures from carbon nanomaterials without apparent limits to their size or shape. As formed tapes or sheets are very robust, fully flexible and offer high tunability in terms of surface microstructure and composition. We believe that they can be a very good platform for gaining greater understanding of science in carbon nanomaterials and bringing them much closer to applications.

A33: Manufacturing methods and properties of 3-dimensional graphitic structures

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The production of 3-dimensional graphitic structures is based on a variety of different process techniques. It can mainly be differentiated into the direct synthesis in a CVD process and assembly methods. In most direct synthesis methods a prestructured template is used that is etched away in a second process step [1]. Few approaches exist to directly synthesize an aerogel without using a template [2]. This method is less effortful but the aerogels have less tailorability. In CVD-based processes a direct covalent interconnection between the growing graphite sheets can be achieved. Using an assembly method beforehand manufactured graphene sheets are formed to a hydrogel by adding crosslinkers with a subsequent freeze drying [4, 5]. The resulting aerogels consist of graphene sheets weakly bonded by van der Waals forces. In this

study we present the method for a direct synthesis of 3-dimensional graphitic structures in the CVD process [3]. In this approach we produce Aerographite by using zinc oxide templates with a tetrapod morphology. In contrary to other template based CVD grown structures, here the underlying template is removed in-situ during the CVD process so that no etching is required. The graphite morphology is dependent on the former template morphology, as it duplicates the former template's surface area. Finally, we show in dependence of the morphology the electric and thermal properties.

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A34: Metallic/semiconducting Separation of SWCNT/H₂O dispersion by Electric-field-induced Layer Formation method

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Recently we have reported Electric-field-induced Layer Formation (ELF) method, which is one of the techniques for the separation of metallic and semiconducting single-wall carbon nanotubes (m- and sc-SWCNTs). Compared with the other separation techniques, the main characteristic of ELF is the applied DC voltage can directly and handily sort the SWCNT dispersion into m- and sc-SWCNTs layers without chromatography media such as gel [1]. Furthermore, it is also characteristic that the surfactant used in ELF is nonionic. The high purity of 98 % was obtained in sc-SWCNT separated by ELF as reported at the last NT15 conference [2]. We normally use D₂O as a dispersion medium in ELF rather than H₂O, because its high density contributes to the better mono-dispersibility and, therefore, the sharpness of separation. However, the cost for D₂O was one of the central concerns in ELF. In this presentation, we report the results of ELF separation using H₂O. SWCNTs synthesized by eDIPS [3] were purified by heat treatment and then dispersed in H₂O solutions of 1 wt% Brij S100 by sonication and ultracentrifugation. By using obtained SWCNT solutions, the comparison study on mono-dispersibility in terms of the ratio of peak intensity in the normalized optical absorption spectra [2] was carried out. Based on the results, the optimal dispersion condition was determined. The SWCNT solution prepared using the optimal condition were separated by ELF method. From the Raman results, the purity of 98% in the sc-SWCNTs fraction was obtained that is the same level of D₂O. As well, the separation cost was extremely reduced to 1/660 by using H₂O. This presentation is based on results obtained from a project subsidized by the New Energy and Industrial Technology Development Organization (NEDO).

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A35: Multilayer graphene on SiO₂: direct formation by "etching-precipitation" and conductivity enhancement by FeCl₃ intercalation

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Manufacturing of graphene films in a controlled fashion is highly desired for the development of electronics technology based on the two-dimensional carbon material with numerous attractive properties. Chemical vapor deposition (CVD) on catalyst metals is now commonly used to synthesize graphene because of its high scalability [1]. However, there are still challenges in developing transfer processes of CVD graphene onto dielectric substrates because this typically leads to deterioration of the material quality. In order to grow graphene films "directly" on dielectric substrates, we previously reported the "etching-precipitation" method [2]. In this method, thin solid solution films of Fe-C are firstly deposited on quartz glass substrates, and then the Fe-C films are exposed to Cl₂/Ar atmosphere at 600–650 °C. This leads to the direct graphene growth on the substrate via precipitation of C. Here, we report our approach to control the layer-number and the electrical conductivity of graphene films grown by the "etching-precipitation" method. We utilize a reactive sputtering technique with a Fe target in C₂H₄/Ar atmosphere in order to deposit Fe-C films. This allows to vary the carbon concentration in Fe-C films (50–100 nm, 17–27 at%C) with C₂H₄ concentration (0.4–0.9 vol%) applied in the deposition at 5 mTorr. We have achieved 230–500 Ω/sq multilayer graphene films with an optical transmittance ranging 56%–80% by adjusting carbon concentrations and thicknesses of the initial Fe-C films. Also, we conduct FeCl₃ intercalation of the resulting graphene samples by sublimating FeCl₃ powder in a closed tubular reactor (Ar atmosphere, 390 Torr) at 340 °C. Our results show that the sheet resistance of graphene gets reduced to 1/5–1/3 by the intercalation, and it is stable for at least ~10 days.

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A36: Nickel endohedral metallofullerenes formation under electron irradiation: experiment and simulation

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Traditional methods of synthesis of endohedral metallofullerenes (EMFs) in the arc discharge reactor or via laser evaporation are limited mostly to alkali earth elements, lanthanides and early transition metals (groups 2 – 4 of the Periodic Table). A new method to produce fullerenes as a result of graphene flake transformation under electron irradiation in HRTEM has been elaborated recently [1]. Here we obtain EMFs with nickel clusters of several tens atoms inside the fullerene shell by electron irradiation treatment in HRTEM of nickel clusters surrounded by amorphous carbon or a graphene flake in the interior of a carbon nanotube. The proposed method can be extended to other late transition metals to produce EMFs with endohedral metal clusters of a given composition and number of atoms including clusters composed from several chemical elements.

To reveal the roles of electron irradiation and carbon nanotube in the formation of EMFs the molecular dynamics simulations using CompuTEM algorithm [2] have been performed for three cases of treatment of nickel cluster surrounded by amorphous carbon: under electron irradiation inside a carbon nanotube, under electron irradiation in vacuum and heat treatment inside the carbon nanotube. Whereas the formation of EMFs is observed for all three simulated cases, the maximum yield of EMFs averaged over simulation runs takes place under electron irradiation inside the carbon nanotube. Thus both the electron irradiation and carbon nanotube promote the EMF formation. Since the yield of EMFs under electron irradiation is several times greater than under heat treatment the role of electron irradiation is essential and related with the transfer of electron kinetic energy mostly to light carbon atoms.

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A37: Nucleation - growth Mode Tuning of Single-Walled Carbon Nanotubes by Regulating the Carburization of Catalyst Particle

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Single-walled carbon nanotubes (SWNTs) have been considered as the likely candidate for miniaturizing nanoelectronics. However, one major obstacle to realization of SWNT-based nanotechnology has been the lack of technique for producing SWNTs with identical structures, mostly due to the incomplete understanding of their formation mechanisms. In this contribution, we demonstrate the reversible modulations of SWNT configurations by regulating the carburization of catalyst particle during chemical vapor deposition (CVD) processes [1]. Particularly, by alternating carbon precursors, including CH₄ and CO, which induce very different carbon chemical potentials at gas-catalyst interface, SWNT intramolecular junctions with significant diameter change along SWNTs are fabricated. By performing a systematic TEM study, the size correlation between the SWNTs and the catalyst

nanoparticles on which SWNTs grow reveals two nucleation modes: perpendicular mode and tangential mode [2], depending on the gas precursor used during CVD. This is because different carbon chemical potentials at gas-metal surface lead to different carbon concentrations in catalyst particle. As demonstrated by Monte Carlo simulations, high carbon content in nanoparticle favors the perpendicular mode of SWNTs nucleation and growth, different from the tangential mode promoted by a low carbon concentration. The calculations are well consistent with the experimental findings, highlighting the importance of particle carburization in controlling the SWNT nucleation mode. Further, TEM analyses reveal that SWNT grown along with the perpendicular mode display selective helicities close to armchair configurations in contrast to tangentially grown SWNTs. These understandings therefore provide guidelines for catalyst design and growth condition optimization, paving the way to success in structure-controlled synthesis of SWNTs.

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A38: Observation of charge generation and transfer during CVD growth of carbon nanotubes

Wang, Jiangtao (Tsinghua University, Beijing, CHN)

Carbon nanotube (CNT) is believed to be the most promising material for next generation IC industries with the prerequisite of a firm chirality specific growth. For various approaches to controlling the chiral indices of CNTs, the key is to deepen the understanding of the catalytic growth mechanism in chemical vapor deposition (CVD). Here we show our discovery that the as-grown CNTs are all negatively charged after Fe-catalyzed CVD process. The extra electrons come from the charge generation and transfer during the growth of CNTs, which indicates that an electrochemical process happens in the surface reaction step. Based on this prospect, we design an in-situ measurement equipment, verifying that the CVD growth of CNTs can be regard as a primary battery system. Furthermore, we find that the variation of the Fermi level in Fe catalysts have a significant impact on the chirality of the CNTs when different external electric fields are applied. These findings not only provide a new perspective on the growth of CNTs but also open up new possibilities for controlling the growth of CNTs by electrochemical methods.

A39: On the change of crowded junctions to bridges p-conjugated systems in the cross-linking of CNTs towards macroscopic materials of enhanced electrical conductivity

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Transfer of CNTs exhibiting a unique combination of physicochemical properties from purely scientific achievements to the every-day life and hence scaled-up applications has yet to be accomplished in numerous areas 1. Individual CNTs represent 1D lightness with high tensile strength, excellent thermal and electrical conductivity 2 while their macro-assemblies typically suffer from deterioration of

properties due to inter-nanotube junctions, van der Waals agglomerates and (aspect ratio)-based discontinuity of conductivity paths 3. While many types of surface CNT modifications reduce the nanotube agglomeration 4, they can introduce unwanted defects in the C-sp²-walls and hence detract their electrical properties 5. It is therefore important to functionalize CNTs with moieties enabling maintenance or possibly enhancement of electrical conductivity in the macroscopic materials. As inspired by organic chemistry methods, we have employed reactions based on the attack of in situ generated phenyl cations and subsequent introductions of π -conjugated bonds able to convey electrons at the inter-nanotube junctions. The so-prepared based on modified CNTs were comprehensively analysed (SEM, TEM, TG, Raman, FT-IR, electrical conductivity) and the results constitute an opening in the chemical construction of CNT-based conductive macro-assemblies.

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A40: One-way burning of single-walled carbon nanotubes from site-controlled nanogaps for full-length removal of metallic nanotubes

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Semiconducting single-walled carbon nanotubes (s-SWNTs) are a great candidate for improving both performance and energy efficiency of logic circuits, due to their excellent electrical properties and ultrathin body. It is necessary to prepare high-density aligned arrays of pure s-SWNTs to maximize the potential. Selective removal of metallic (m-) SWNTs from as-grown SWNT arrays has not offered sufficient selectivity, applicability to high-density arrays, and scalability to large circuits at the same time. We recently reported polymer- and water-assisted burning of m-SWNTs triggered by Joule self-heating [1]. This reproducibly resulted in long-length removal of m-SWNTs, though the burning length still had wide distribution. We first fabricated multiple field-effect transistors (FETs) by adding electrodes at the middle of the SWNT arrays purified by water-assisted burning. FETs on one side successfully showed high on/off ratio, while FETs on the other side did not. This suggests bias voltage dependency of the burning region. We revealed that this asymmetry originates from one-way burning of SWNTs from initial breakdown position, probably triggered by field electron emission from the SWNT tips [2]. Therefore, the burning length solely depends on the randomly scattered breakdown position. To further improve the burning length, we controlled breakdown location by partially suspending SWNTs over trenches, where heat dissipation from SWNTs was suppressed. Larger burning length with narrower distribution was achieved ($92 \pm 13\%$ of full length; $\sim 10 \mu\text{m}$) compared to uncontrolled breakdown ($54 \pm 26\%$).

Suspension over trenches also enables the breakdown at lower voltage, and can avoid the breakdown of s-SWNTs.

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A41: Prussian blue and Prussian blue analog nanoparticles as catalyst precursors for chemical vapor deposition growth of single-wall carbon nanotubes

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The unique electronic properties of SWCNTs, which make them a promising candidate for applications in nano-sized electronic devices, are directly related to their atomic structure [1]. Achieving chiral-selective growth of SWCNTs is therefore a key element to exploit their properties to their full potential [2]. It has been observed that using bimetallic catalyst nanoparticles can increase the selectivity of SWCNT growth [3]. In this study, we investigate the effect of bimetallicity by comparing SWCNT growths using two different catalysts: pure iron, and bimetallic NiFe. The catalyst nanoparticles are obtained by a reductive treatment of Prussian Blue (BP) and NiFe Prussian Blue analog (PBA) nanoparticles, respectively. We employ a versatile multistep fabrication process based on coordination chemistry and surface chemistry that allows us to control the dispersion of the catalyst particles on the sample surface [4]. A SiO₂ substrate is coated with a self-assembled monolayer (SAM) of an organic ligand, and dipped into a dispersion of PB nanoparticles. The particles attach to the substrate by coordination bond with the organic SAM. The pre-catalyst particles are then converted into active metallic/bimetallic catalysts, followed by hot filament CVD growth. The catalyst size distributions are determined by transmission electron microscopy (TEM), and their composition is studied by energy dispersive X-ray spectroscopy (EDS). Diameter distribution of SWCNTs is studied by coupling resonant Raman spectroscopy with four wavelengths and TEM. Raman spectroscopy allows the comparison of the selectivity for the different SWCNT growths, by determination of the semi-conductor to metallic ratio.

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A42: Purity Improvement of Semiconducting CNT Ink Using Multi-Step Elution Chromatography

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Semiconducting carbon nanotubes (S-CNTs) are promising material for various applications especially for flexible electronic devices. For the practical application of S-CNT, development of high-quality and low-cost S-CNT ink is very important, because it can be used for printing electronics without any additional treatment. In this work, we have developed an improved S-CNT ink preparation method using a gel column chromatography. This method realized extremely high-purity S-CNT ink, which can highly improve the stability and transfer characteristics of thin film transistors. Usually, in the presence of sodium dodecyl sulfate (SDS), S-CNTs are adsorbed on the dextran-based gel and then eluted by deoxycholate (DOC). In the previous method, high concentration DOC eluted S-CNTs with various diameters. In this work, we have increased the DOC concentration step by step in the elution process (multi-step elution). In this case, S-CNTs were eluted sequentially from thin-to thick-S-CNTs. Furthermore, in the several fractions, the purity of S-CNT was found to be highly improved. S-CNT ink was then prepared by replacing the surfactant to nonionic one, which showed highly stable transistor performances. This presentation is based on results obtained from a project commissioned by the New Energy and Industrial technology Development Organization (NEDO).

A43: Scalable technology for fabrication of clean and durable electrical contacts between individual substrate-supported SWCNTs and metal leads

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Exploitation of exciting properties of individual single-walled carbon nanotubes (iSWCNT) in electronic devices is often hindered by their low quality contacts to metal leads. Here we present a scalable process for fabrication of carbon nanotube field-effect transistors (CNFETs) with iSWCNTs as device channels. The approach is developed based on a combination of using sacrificial layer and plasma oxidation as well as utilization of thin Cr adhesion layer prior to noble metal deposition for electrical contacts. The electrical contacts of CNFETs fabricated with this process reveal low median on-resistance and long lifetime. In this approach SWCNTs are synthesized directly at predefined areas by CVD process [1]. As-grown SWCNTs are covered by Al₂O₃ sacrificial layer deposited by ALD to prohibit their direct exposition to resist [2] and to protect them from the impact of plasma ashing. Al₂O₃ layers

thicker than 18 nm can sufficiently protect SWCNT from the impact of 100W oxygen plasma as proved by CNFET electrical measurements and SWCNT Raman spectroscopy. Plasma oxidation is applied to remove photoresist residuals from contact areas. Sacrificial alumina layer is removed by H_3PO_4 exposure prior to contact metallization. This is a residue-free process step with no detectable influence on properties of SWCNTs [2]. The median on-resistances of 959 Cr/Au-contacted CNFETs fabricated on the Si/SiO₂ wafer were determined to be 89 kOhm [3]. We observed lifetime of devices exceeding 90 days even for non-passivated CNFETs using a Cr layer below 2 nm in Cr/Au contacts [4].

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A44: Self-loop synthesis of highly conductive mesoporous graphene frameworks and their superior performance as cathode scaffolds for lithium-sulfur batteries

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With the development of portable electronics, batteries systems especially lithium-sulfur batteries have drawn increasing attention in recent years due to their ultrahigh theoretical energy density of 2600 W h g⁻¹. Considering the insulation of sulfur, many efforts have been dedicated to exploring a cathode scaffold based on nanocarbon materials to accommodate and fully utilize sulfur for lithium-sulfur batteries. Among various options, porous graphene, which usually has a high electrical conductivity along with hierarchical porous architectures, is a promising candidate. Notwithstanding the advances of several hard templates being employed to fabricate porous graphene via chemical vapor deposition (CVD) process, careful structure modulation of the products based on templates is still few touched, a scalable and controllable synthesis route for such templates also needs to be developed. Herein we proposed a facile way to fabricate mesoporous graphene frameworks (MGFs) through CVD of CH₄ on MgO templates. These MgO templates could be easily regenerated by a precipitation step, and via modulating the template-precursors as well as the templates themselves, structures and properties of MGFs based on them were also well tuned. Eventually, a high surface area of 2032 m² g⁻¹, a pore volume of 2.99 cm³ g⁻¹ besides a high electrical conductivity of 66.5 S cm⁻¹ was achieved for the MGFs serving as cathode scaffolds in lithium-sulfur batteries. Electrochemical evaluation demonstrated extraordinary cycling stability and rate performance: the MGF-S cathode delivered a high initial discharge capacity of 1384 mAh g⁻¹ at the current rate of 1.0 C. Even after 100 cycles, a relatively high capacity of 977 mAh g⁻¹ was still retained, with the Coulombic efficiency constants at about 97.0 %. Such a simple method offered a general strategy for the bulk synthesis of advanced carbon

nanomaterials applied extensively in the area of energy storage. Keywords: mesoporous graphene; template modulation; cathode scaffold; lithium-sulfur batteries.

A45: Structure sorting of large-diameter carbon nanotubes by NaOH tuning the interaction between nanotubes and gel

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Structure sorting of single-wall carbon nanotubes (SWCNTs) into mono-chiral species is critical for their property study and application in devices. Recently, gel chromatography has been demonstrated to be a simple and high-efficiency technique for the single-structure separation of small-diameter SWCNTs (diameter less than 1.1 nm), but it still faces the challenges in separating the SWCNTs with diameters larger than 1.1 nm. Here, we report that the structure separation of the SWCNTs with diameters ranging from 1.2 to 1.7 nm has been achieved by NaOH tuning the interaction between the nanotubes and gel. In the gel chromatography technique, sodium dodecyl sulfate (SDS) is usually used as surfactants for the dispersion of nanotubes. However, the hydrolysis of SDS molecules would produce H⁺ ions, which prefer to adsorb onto the large-diameter nanotubes. The adsorption of H⁺ ions on the nanotube surfaces could screen the columbic interaction between the negative charges at the end of SDS molecules, resulting in an increase in the density of SDS molecules on the nanotube surfaces and thus a decrease in their adsorb-ability onto the gel. The reducing adsorbability would inevitably decrease the interaction difference of various large-diameter nanotubes with the gel. The introduction of NaOH could selectively neutralize the H⁺ ions on the nanotube surfaces and thus reduce their screening effect, leading to amplifying the interaction difference of the different nanotubes with gel, and achieving their structure separation. The present results extend the ability of the gel chromatography technique in recognizing and separating structures of large-diameter SWCNTs.

A46: Synthesis and applications of kilometres of continuous macroscopic fibres with controlled type of carbon nanotubes and bundle orientation

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We report on the synthesis of kilometres of continuous macroscopic fibres made up of carbon nanotubes (CNT) of controlled number of layers, ranging from singlewalled(SW) to multiwalled(MW), tailored by the addition of sulfur as a catalyst promoter during CVD in the direct fibre spinning process[1]. The progressive

transition from SW through collapsed double-walled to MW is clearly seen by an upshift in the 2D (G') band and by other Raman spectra features. The increase in number of CNT layers and inner diameter results in a higher fibre macroscopic linear density and greater reaction yield (up to 9%). We establish the composition of the catalyst particles and position in the isothermal section of the C – Fe – S ternary diagram at 1400 ° C. This helps explain the unusually low proportion of active catalyst particles in the direct spinning process (<0.1%) and the role of S in limiting C diffusion and resulting in catalyst particles not being in thermodynamic equilibrium with solid carbon, therefore producing graphitic edge growth instead of encapsulation[2]. We further present the distribution of CNT chiralities obtained from ED, Raman and Emission spectra, showing the predominance of metallic SWNTs. This biased is discussed in the context of the current screw dislocation growth model accepted in the field[3]. Finally, we show the application of basic polymer fibre spinning principles to produce highly oriented CNT fibres by reducing entanglements in the gas phase through CNT dilution[4]. The resulting fibres have tensile properties superior to those of Kevlar, high electrical conductivity and a very large surface area. The exploitation of these properties in sensors, supercapacitors and other devices is briefly demonstrated[5].

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A47: Synthesis of Chirality Specific Single-Walled Carbon nanotubes

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It is well known that small changes in the diameter and chiral indices (n, m) of single-walled carbon nanotubes (SWNTs) will change the bandgap. Therefore, the production of just one type of SWNT by controlling its structure during growth is an important goal. Here we show, that by using the protocol described by Yan Li et.al in 2014, we have produced template growth of SWNTs with a specific (n, m) by using a range of new nanocrystal catalysts synthesized in our laboratory.

A48: Synthesis Of Single Walled Carbon Nanotube (Swnts) With Specified Electric Properties For Nano Electronic Applications

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In this work we present a robust and versatile approach for the reproducible and controllable growth of single wall carbon nanotubes (SWNTs) through a self-assembled monolayer (SAM) technique coupled with an atomic hydrogen (Hat) pretreatment to control the catalytic metallic nanoparticles size and density. SWNTs exhibit a remarkably good crystalline quality, with a diameter (and type) strongly dependent on the nature of the initial catalyst precursor and its preparation. Field effect transistors (FETs) with excellent characteristics were obtained using such in-place grown SWNTs. The electronic properties of the SWNTs can be tuned: the transistors obtained from Ru(TPP) and FeCl₃ exhibit I_{ON}/I_{OFF} current ratio up to $\sim 10^9$, indicative of the direct growth of a high proportion of semiconducting nanotubes over than 98%. Such elevated values have been reported essentially for CNT-FETs devices based on individual semiconducting SWNTs.

A49: The Effect Of Using Natural Gelling Agents In The Properties Of The Graphene Aerogels

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The purpose of this work is the preparation of graphene aerogels using natural gelling agents and graphene oxide (GO). The graphene aerogel is a three dimensional structure (3D) with high porosity and low density. Pore sizes are as large as several tens of microns, which allow easy access and diffusion of ions and molecules across the structure. These 3D graphene structures maintain their accessibility to their effective surface area by keeping graphene nanosheets as individual as possible, which is essential for achieving maximum functionality of macroscopic graphene-based materials. As a result, they have found a lot of promising applications for these materials as: catalysts, flexible sensors, nanocomposites with high electrical conductivity, storage and conversion of energy, oil absorption, water purification, etc. We used gelatine and L-ascorbic acid as gelling agents. Both compounds are biodegradable and biocompatible natural chemical products. After FTIR and Raman analysis, one interesting finding is that gelatine as well as L-ascorbic acid are both acting like good reduction agents. This fact is of great importance since it helps to substitute thermal reduction that tend to collapse the aerogel structure by the abrupt removal of the functional group, compromising the 3D structure and the mechanical properties of the final material. SEM images show the porous structure of the graphene aerogel obtained using natural gelling agents, it is possible to observe that the graphene aerogel synthesized with L-ascorbic acid show smaller porosity structure than gelatine compound. The surface area of the aerogel was characterized using nitrogen chemisorption.

A50: The importance of electrical current in post-synthetic crystallization process for the improvement of single walled carbon nanotubes properties

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Defects in the carbon nanotubes (CNTs) represent a bottleneck for harnessing their full potential in applications. Many properties, such as electrical and thermal conductivities, are highly sensitive to the presence of crystalline defects in CNT and, in particular, single-walled carbon nanotubes (SWCNTs), where the entire structure is composed of a single layer of graphene [1]. While post-synthetic processes have been proposed using the direct application of heat have demonstrated increase in crystallinity, coalescence of SWCNTs into double-walled CNTs have been reported [2]. In this study, we developed an original post-synthetic process (*heat and current process*) to remove the defects in SWCNTs while retaining the diameter and wall number. This was achieved by applying electrical current (current density: $\sim 240 \text{ A cm}^{-2}$, electrical power density: $\sim 2000 \text{ W cm}^{-2}$) in conjunction with heating ($\sim 2000 \text{ }^\circ\text{C}$) to a “aligned SWCNT sheet.” At $800 \text{ }^\circ\text{C}$, 150 A cm^{-2} (1150 W cm^{-2}) for 1 min, we achieved a 3.2-times increase in the Raman G- to D-band ratio, a 3.1-times increase in electrical conductivity (from 25.2 to 78.1 S cm^{-1}), and a 3.7-times increase in thermal conductivity (from 3.5 to $12.8 \text{ W m}^{-1} \text{ K}^{-1}$). The electrical and thermal conductivities did not only increase simultaneously, but their relative increases were identical across our experimental range that stems from defect healing without any change in diameter and wall number. In contrast, a significant increase in diameter and wall number was observed when current was not applied at high temperature. These results demonstrate the importance of applying current to improve the graphitization of SWCNTs while maintaining their structure as SWCNTs. We believe that this process overcomes one of the major limitations of SWCNTs toward real application. This study is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO). [1] N. Matsumoto et al., *Nanoscale* 87 (2015) 239. [2] N. Matsumoto et al., *Carbon* 7 (2015) 5126.

A51: The Internal Buckling Behavior Induced by Growth Self-restriction in Vertical Multi-walled Carbon Nanotube Arrays

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In general, the internal buckling is ubiquitous in the grown CNT arrays. It is an important factor which makes the measured physical properties of carbon nanotube array lower than that calculated in theory. In this work, the evolution and fabrication mechanism of the internal buckling in the vertically grown carbon nanotube arrays have been studied systematically. The internal buckling of CNTs was induced due to the self-restriction process in the grown CNTs. Considering lateral deviation, we generalized the Euler beam to wave-like beam, and built the model from quasi-static compression which was applied to analyze buckling behavior in carbon nanotube arrays. The calculated results, which were proofed by Raman spectroscopy, confirmed the change rule of internal interaction between carbon nanotubes with different real length. Basing on these, we prepared well-organized carbon nanotube array in local via adjustment of experimental method.

A52: Transparent and Conductive Hybrid Graphene/Carbon Nanotube Films

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Carbon nanomaterials (carbon nanotubes (CNTs) and graphene) are promising materials for optoelectronic applications, including flexible transparent and conductive films (TCFs) due to their extraordinary electrical, optical and mechanical properties. However, the performance of CNT- or graphene-only TCFs still needs to be improved. One way to enhance the optoelectrical properties of TCFs is to hybridize CNTs and graphene. This approach leads to creation of a novel material that exhibits better properties than its individual constituents. In this work, the novel hybrid CNT-graphene nanomaterial was fabricated by graphene oxide deposition on top of CNT films. The graphene oxide was then reduced by thermal annealing at ambient atmosphere or in H₂ atmosphere. At the final step the CNT-graphene hybrids were chemically doped using gold(III) chloride. As a result, we show that the hybrids demonstrate excellent optoelectrical performance with the sheet resistance as low as 73 Ohm/sq. at 90% transmittance. This research was supported by the Ministry of Education and Science of Russian Federation under the grant agreement no. 1425320 (Project DOI: RFMEFI58114X0006).

A53: Wafer-scale synthesis of chiral-consistent monochromatic ultralong carbon nanotubes

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Many products have been realized based on carbon nanotubes (CNTs) despite of insufficient use of their extreme performances owing to defects in structure. In contrast, ultralong CNTs possess theoretical properties of CNTs with macroscale length, atomically consistent perfect structure and superior properties, exhibiting intriguing potential in the next-generation high-end electronics. But a great challenge to realize large-scale application is controllable wafer-scale synthesis of ultralong CNTs. In this work, we have designed a new layered cuboid reactor (LCR) and replaced the original tube furnace with a larger muffle furnace with $1000 \times 300 \times 300$ mm³ in size, which optimized the traditional chemical vapor deposition system and released the restriction of short heating zone and small-sized substrates. With longer preheating zone, multiple commutating zone and larger growth area in design, LCR has an enlarged invariable temperature area and more uniform gas velocity distribution, favorable for wafer-scale synthesis of ultralong CNTs and more than five 4-inch wafers of ultralong CNTs were firstly synthesized simultaneously. Ultralong CNTs on these wafers could be directly observed by naked eyes in ambient conditions assisted with condensed vapor, avoiding the size constraints for samples under normal electron microscope. Furthermore, Raman spectra and Rayleigh scattering demonstrated the perfect structure of as-prepared ultralong CNTs with consistent chirality. Field effect transistors fabricated from as-prepared ultralong CNTs exhibited a high on/off ratio of 10^7 , associated with the semiconducting properties and structure perfectness of ultralong CNTs. This creatively-designed system with LCR will provide a scalable and effective route to synthesize larger-area ultralong CNTs or two-dimensional nanomaterials, enabling large-scale integrated circuits and other optoelectronic applications in the future.

POSTER SESSION B: Sensors & Devices

B1: Carbon nanotubes in high magnetic field

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A parallel magnetic field affects strongly the electronic transport through a carbon nanotube (CNT) via its coupling to the orbital degree of freedom. Although such a wire-like system can host neither the fully developed Hofstadter butterflies nor Landau levels, the magnetic field has nevertheless a deep influence on the CNT's spectrum and wave functions. We report here on the results of both theoretical calculations and experimental measurements of a CNT quantum dot. The two experimental results on which we focus are a strong suppression of the conductance by the parallel magnetic field and an unusual evolution of the spectral lines. The unique boundary conditions, which couple the transverse and longitudinal momentum, are responsible both for decreased transmission through the CNT and for the unexpected dependence of the longitudinal momentum on the magnetic field.

B2: Chain-less CNT-FETs for a competitive wafer-level sensor technology

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Single-walled carbon nanotubes (SWCNTs) show unique mechanical properties like high young's modulus and giant piezoresistivity, which make them a promising material for strain sensing applications. Aiming a scalable technology for fabrication of such electro-mechanical CNT sensors, it is mandatory to control the SWCNT assembly structure by prevention of SWCNT chain formation in the transistor channel. Since this chain formation is mainly determined by the length distribution of the SWCNT material, the pre-selection according to length is a prerequisite for successful device fabrication. Here we present recent highlights from length-separation of type-enriched semiconducting SWCNTs by size-exclusion chromatography and its impacts on the structural and electrical CNT-FET properties statistically and comparatively evaluated. It is found that the integration of long SWCNTs significantly suppresses the formation of SWCNT chains and favors homogeneous SWCNT assemblies. The integration yield, defined by number of working transistors over measured transistors, is significantly increased from 71.4 % to 95.2 % by integrating long SWCNTs instead of short SWCNTs. While I_{On}/I_{Off} distribution of CNT-FETs is elevated for short SWCNTs, which can be explained by suppression of conductive channels due to chain formation, integrating long SWCNTs leads to improved performance in terms of hole-mobility μ and subthreshold swing S . The mobility is found to be highest for long CNT-FETs with μ up to 291.9 cm²/Vs and

decreases to 127.5 cm²/Vs and 61.5 cm²/Vs for reference and short SWCNTs, respectively. Moreover CNT-FETs consisting only of long SWCNTs exhibit better controllability with significant reduction of the subthreshold swing compared to reference and short CNT-FETs.

B3: CNT sheets as aligning electrodes for liquid crystal displays

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Liquid crystals (LC) have attractive electro-optic properties successfully used in displays and other optoelectronic applications. Prerequisite for such uses is the achievement of uniform alignment of LC molecules and this can be easily obtained by confinement of the LC between two surfaces suitably treated, typically with rubbed polyimide. The substrates are equipped with indium tin oxide (ITO), a transparent electrode to let the light be transmitted through the LC filled cell and, at the same time, to apply electric fields for changing the orientation of LC molecules. The existing alignment layers present some problems like possible contaminations in the LC and cost. As attractive alternative for aligning LCs we present the use of carbon nanotube (CNT) sheets that are also interesting as conductive and transparent electrodes.

A single sheet of aligned multi-wall CNTs, obtained by pulling the tubes from forests, was deposited on a glass substrate and then coated with SiO₂. Two similar substrates were glued together forming a gap filled by capillarity by the nematic liquid crystal 5CB (4'-Pentyl-4-biphenylcarbonitrile). The alignment of LC was assessed by Polarized Optical Microscopy finding a stable, uniformly planar and unidirectional orientation. By applying to the CNT sheets voltages above a certain threshold value the reorientation of the LC molecules could be obtained with the subsequent change in the optical properties, achieving electro-optic modulation. The behaviour of the LC in presence of the CNT sheet-equipped cell was investigated as function of temperature and fields.

Our results indicate that the CNT sheets are promising multifunctional layers for LC displays combining different functionalities, allowing to skip preparation steps and materials and, at the same time, offering attractive performance.

B4: Demonstration of terahertz sensing and imaging with carbon nanotube devices

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Imaging technologies based on terahertz (THz) frequency waves are increasingly expected as a powerful tool for non-destructive inspection, especially in the fields of security, organic/inorganic materials characterization, agriculture, medical and biological sciences. In order to realize THz technologies for practical use, high-sensitive and wide-band THz detectors, working even at room temperature, are in strong demand. THz photon energy, however, is much lower than the thermal energy

at 300K (26 meV), making it difficult to detect THz waves at room temperature via conventional techniques. Here we report on a novel THz detector based on photothermoelectric effect of carbon nanotubes. Owing to their unique band structure, carbon nanotubes have strong advantages such as high conductivity, mechanical strength and ultra-wide band absorption from DC to ultraviolet light. On this basis, we achieved room temperature THz detection with carbon nanotube devices, ranging over a wide frequency band from 0.14 THz to 30 THz. Additionally, we found strong dependence on electrode metals, revealing the detailed mechanism of the photothermoelectric effect occurring at the interface between carbon nanotubes and electrodes. The findings enabled us to miniaturize the detector size while keeping the detection sensitivity. By utilizing a compact carbon nanotube THz sensor, we demonstrated THz imaging of metals concealed behind an invisible object, which is expected to bring a large spillover effect on non-destructive and non-contact inspections in the future.

B5: Effect of inhomogeneous charge localization in target molecules on biosensor response using carbon nanotube thin film transistor

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Label-free electrochemical sensing using carbon nanotube thin film transistors (CNT-TFTs) is one of the most promising ways for rapid and highly sensitive monitoring of biomolecules because CNT has excellent electric properties, a large surface and stability against chemical reactions. In sensing, the specific biomolecules with charge are adsorbed on the channel surface using antigen-antibody reaction, and change of the charge within the Debye length is detected as the sensor response. If total charge of adsorbed molecules within the Debye length is a negative, the source-drain current (I_{sd}) in the transistor as a sensor response increases by modulating the surface potential. In general, the biomolecules don't fall within the Debye length (several-nm) of standard sensing conditions. Furthermore the large biomolecules have inhomogeneous charge distribution. The charge inhomogeneity in the biomolecules should affect the sensor response critically, but it has been neglected in past reports. In this study, we analyzed the sensor response from CNT-TFTs with adsorption of immunoglobulin E (IgE) by varying Debye length (3-90nm). IgE is large molecule (~188 kDa) and its y-shape is supposed to cause biased charge distribution: a part of the antigen-binding fragment where binds to IgE aptamer has a positive charge, and the whole antibody of IgE has a negative charge. When the Debye length was 3nm, the I_{sd} in CNT-TFT increased with increasing IgE concentration up to nM order of the IgE concentration, and the I_{sd} suddenly decreased at over several hundred nM. When the Debye length was 90 nm, I_{sd} increased consistently from 500 fM to 500 nM. The complicated response observed for different Debye length are originated from configuration of adsorbed IgE molecules and consequently their net charges falling within the Debye length. This result indicates that large biomolecules are detected quantitatively by optimizing the Debye length and considering the effect of steric hindrance.

B6: Electrical and mechanical properties of single-walled carbon nanotube fibers based on various carbon nanotube dispersed solutions by wet spinning

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For fabricating continuous carbon nanotube (CNT) fiber, wet spinning, CNT dispersed solution injecting into a coagulating solution, is well known method. Recently, we develop polymer-free CNT fibers with high electrical and mechanical properties by wet spinning. Successful fabrication of continuous CNT fibers requires a balance between the dispersibility of CNTs in a solvent, and the cohesive attraction among the CNTs. The tradeoff between the dispersibility of CNTs and the cohesive attraction among them can be controlled by the sonication times or types of surfactants. Here we report electrical and mechanical properties of polymer-free CNT fibers based on various CNT dispersed solutions where the dispersibility of CNTs varied by sonication time and types of surfactants [1,2]. This paper is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO). 1. K. Mukai, K. Asaka X. Wu, T. Morimoto, T. Okazaki, T. Saito, M. Yumura, submitted. 2. X. Wu, T. Morimoto, K. Mukai, K. Asaka, T. Okazaki, submitted.

B7: Fabrication and characterization of all-carbon nanotube thin-film transistors on stretchable substrates

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Flexible and stretchable electronics have been intensively explored for wearable and bioimplantable applications such as electronic-skins and healthcare/medical devices. Carbon nanotube (CNT) thin-films are a promising candidate for their applications due to their excellent carrier mobility, mechanical flexibility, transparency and chemical stability. In addition, CNT thin-film can be used both as a metallic conductor and as a channel material for high-performance transistors [1], which enables to fabricate the high-performance and transparent all-carbon devices providing a possibility of realizing wearable devices without feeling its existence. In this work, we have fabricated stretchable and transparent all-CNT transistors on poly(dimethylsiloxane) (PDMS) substrates. The uniaxial stretching test have also been performed. The device fabrication was carried out on a Si substrate, and subsequently the devices were transferred on a PDMS substrate. The CNT electrodes were formed by the dry transfer process based on the floating-catalyst CVD [2] and subsequent photolithography process. Semiconducting CNTs purified by the gel chromatography [3] were used as the channel material. One-dimensional tensile strain test showed a small degradation in drain current as 8 % under the tensile strain

of 20%. We also confirmed that the device worked even for 40% tensile strain, and the drain current returned to the initial value when the strain was released. [1] D.-M. Sun et al., *Nature Nanotechnol.* 6, 156 (2011). [2] A. Kaskela et al., *Nano Lett.* 10, 4349 (2010). [3] T. Tanaka et al., *Appl. Phys. Express* 1, 114001 (2008).

B8: Highly flexible and extremely high-gain complementary inverters of transition metal dichalcogenide monolayers

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Monolayer transition metal dichalcogenides (TMDCs) have attracted much attention because of their large bandgap and atomically thin thicknesses and are promising semiconducting materials for future electronics. Currently, using the chemical vapor deposition (CVD) method, we synthesized various large-area TMDC monolayers and fabricated electric double layer transistors (EDLTs) in which the dielectric layers of transistors are replaced with EDLs of electrolytes.[1-8] Owing to the high specific capacitance of EDLs (1-10 $\mu\text{F}/\text{cm}^2$), EDLTs can continuously control carrier density up to $5 \times 10^{13} \text{ cm}^{-2}$, which results in the tuning of the transistor polarity between p-type and n-type. Moreover, the CVD-grown large-area TMDC monolayer EDLTs achieved a high mobility ($\sim 100 \text{ cm}^2/\text{Vs}$), high on/off ratio ($\sim 10^6$), and low S ($\sim 60 \text{ mV}/\text{dec}$). In this study, we demonstrate CMOS inverters using large-area TMDC monolayers. By combining p-type WSe_2 and n-type MoS_2 EDLTs, we fabricate CMOS inverters with the highest voltage gain among the 2D materials (~ 110), with negligible off-state voltage, large total noise margin ($> 95\%$), low power consumption ($< 200 \text{ pW}$), and good switching speed ($> 1 \text{ kHz}$). Moreover, we transfer these inverters onto plastic substrates and evaluate their bendability. The inverters on flexible substrates exhibit stable operation, even when the devices were bent to a curvature radius of 0.5 mm, thereby demonstrating highly flexible CMOS inverters of large-area TMDCs.

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B9: In-situ polymerization of carbon nanotube based field-effect transistors

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In order to exploit the whole potential of single-walled carbon nanotubes (CNT) in devices such as multi-tube field-effect transistors (FET), it is of crucial importance to have control over the CNTs assembly in order to avoid performance limiting effects such as gate screening caused by strong inter tube coulomb interactions. We present a novel post-processing approach enabling a manipulation of the FET channel properties via in-situ polymerization by self-initiated photografting and photopolymerization using vinylpyridine and styrenesulfonate monomers. The impact of the polymerization process was analysed by means of electrical characterization and Raman spectroscopy. We show that this approach allows to improve significantly CNT-FET properties. In particular, the on-off ratios were enhanced by up to four orders of magnitude. Evenly the on-conductance and hole mobility increased. Additionally, a reduced variability, long-time stability and ambipolarity can be reported. Furthermore, the nature of the occurring hysteresis in the transfer characteristics changed from a counterclockwise to a clockwise direction. In order to fully understand those processes, comprehensive investigation are going to be discussed in detail emphasising especially the CNT-bundling issues as well as a change of the direct environment of the CNTs.

B10: Integration of CNTs aligning electrodes in liquid crystal cells

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The alignment of liquid crystal (LC) can be generally achieved by simply treating surfaces on which the molecules anchor and assume a specific orientation, transferred to the neighbour LC molecules finally obtaining a bulk alignment. The common processes used for realizing the aligning surfaces are based on rubbing polymer films that coat glass substrates. Among the alternative methods also carbon nanotubes (CNTs), deposited on substrates showed to be able to orient LC [1]. Here we use a single sheet of aligned CNTs [2] for orienting LC molecules and also as electrodes for applying electric fields to change LC orientation. Single sheets of CNTs were deposited on substrates and the quality of the alignment of the tubes turned out to be important for the LC macroscopic order. The adhesion of CNTs on the substrates is critical otherwise some tubes can detach and mix in the LC deteriorating the liquid crystal display performance. In order to promote the adhesion, the surfaces were silanized for enhancing the hydrophobicity by Hexamethyldisilazane (HDMS). To improve the performance a dielectric layer of SiO₂ was deposited on the CNTs-coated substrates by the e-beam evaporation method, obtaining stability for the multilayer stack. The characteristics and uniformity of the CNTs/SiO₂ layers were investigated by SEM and AFM. The effects of the additional layers on the LC were evaluated by analyzing the texture with Polarizing Optical Microscopy and monitoring the switching behaviour by electric fields. The optical anisotropy of the CNTs-coated substrate was investigated by measuring the optical absorption parallel and perpendicular to the CNT aligning direction.

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B11: Length-dependent performance of single-wall carbon nanotube thin film transistors

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The random networks of single-wall carbon nanotube (SWCNT) have been used as channels of thin film transistors (TFTs). The electronic transport mechanism of SWCNT–TFTs roughly follows the percolation theory. However, as the non-negligible factors, the structure of individual SWCNTs and morphology of SWCNT networks are also important for understanding the electronic transport properties of SWCNT–TFTs.

Recently, we had reported SWCNT-TFTs using mono-dispersed and length-sorted SWCNTs prepared by DNA wrapping and size exclusion chromatography (SEC)¹. By using this method, homogeneous SWCNT networks were formed and high on/off ratio were obtained by controlling of the SWCNT density according to the percolation theory even though the electric property of SWCNTs was still unseparated. The SWCNT length is related to the percolation threshold and should affect the total contact resistances between SWCNTs. In this study, we have fabricated the SWCNT–TFTs with length-sorted SWCNTs with various length distributions to clarify the detailed effects of SWCNT length on the performance of SWCNT–TFTs. Furthermore, we have normalized SWCNT density using a percolation threshold and compared TFT performance between different SWCNT lengths on the basis of the normalized density. From the results of this study, higher performances were obtained in longer SWCNTs and it was found that the average SWCNTs length is an important factor to determine the device performance. Furthermore, detailed analyses confirmed that the effect of SWCNT length on the performance of SWCNT–TFTs clearly appeared in the variations of off-state properties.

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B12: Magnetic field control of the electron-vibron coupling in a carbon nanotube quantum dot

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Quantum dots in suspended single wall carbon nanotubes define a prototypical nano-electromechanical system: the quantized harmonic oscillator behaviour of the longitudinal vibration mode becomes clearly visible in low-temperature transport spectroscopy. Here, we present measurements on a nanotube device tuned to the region of $0 \leq N \leq 2$ trapped electrons, i.e., close to the electronic band gap. A highly localized electronic system in strong Coulomb blockade is present. At finite bias, we demonstrate the emergence of Franck-Condon side bands in single electron tunneling, corresponding to the longitudinal vibration, solely in a magnetic field

along the carbon nanotube axis. The magnetic field evolution of the Franck-Condon coupling factor g is analyzed. For the two-electron ground state it increases from $g=0$ starting at $B \approx 1.5\text{T}$ and reaches a maximum around $B \approx 3.3\text{T}$, however, for different electronic quantum states differing vibronic side band behaviour is found. We present tentative models, based on the influence of axial magnetic fields on the localization of the electronic wave function. The impact of spin / valley quantum numbers on the electron-vibron coupling is discussed.

B13: Spray-coated carbon nanotube film for ammonia gas sensing

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To investigate their use as an NH_3 gas sensor, multiwalled carbon nanotubes (MWCNTs) were deposited on polyethylene terephthalate (PET) substrates using a spray coating technique. Sodium dodecyl sulphate (SDS) was used as surfactant to disperse the nanotubes uniformly in deionized water and then to deposit them on the PET film without the support of an adhesive layer. Chemical treatment with HNO_3 was applied to improve the gas sensing properties by removing SDS, followed by annealing for 1 hr at 100°C . Different characterization techniques such as Raman spectroscopy, scanning electron microscopy and transmission electron microscopy were employed to study the crystal structure and morphology of the nanotube material. A semiconductor characterization system (Keithley 4000-SCS) was used to measure the electrical properties of the gas sensor. The change in the DC resistance of the MWCNT film due to exposure to NH_3 gas in the 50-100 ppm range was recorded. The electronic circuitry of the sensor was designed and fabricated on a bread board to evaluate the sensor performance. The response and recovery times were found to be 1 and 10 min, respectively. The results were well reproducible, demonstrating the potential of using a MWCNT film as gas sensor.

B14: Wafer-level technology platform for manufacturing of high performance CNT devices in electronics and sensors

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Without doubt Carbon Nanotubes (CNT) are extremely interesting for various applications. However, making use of the intrinsic properties with industrial compatible integration technologies remains extremely challenging. The Carbon Path in the cluster of excellence Center for Advancing Electronics Dresden (cfaed) gives a contribution to this open topic by the development of a modeling and technology platform enabling high performance devices such high-frequency CNT field-effect transistors. Therefore, we combine the extensive and complementary multi-disciplinary CNT-FET competences in Dresden and Chemnitz covering materials

science, multi-scale device modeling, RF circuit design and fabrication, and wireless communications. We are going to give an overview about our platform and recent highlights. For guiding the technology development and for enabling circuit design studies, an experimentally verified multiscale simulation framework for CNTFETs covering all levels from atomistic simulations, to TCAD simulation up to compact models has been established. Beside contact studies, the multiscale simulation framework allows the study of defects and different transport phenomena at different channel length scales from a few nanometer up to several micrometer length. On the technology site, we present advanced approaches for channel engineering covering the integration of length-separated CNTs as well as a novel in-situ post-polymerization procedure enabling significant transistor performance enhancements. Based on statistical studies on large FET arrays we demonstrate a comparative study on different post-treatments of FETs in order to tackle contact and hysteresis issues. Moreover, the progress on understanding and controlling of CNT assembly on wafer-level is presented. Finally, we demonstrate TCAD optimized high frequency CNT-FETs fabricated on wafer scale. Equally, we also show recent achievements on electro-mechanical systems with wafer-level integrated CNTs.

B15: A new directly placement method for CNT and strongly-coupled nanotube electromechanical resonators

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Though carbon nanotube is acknowledged as an ideal system for one-dimensional physics, making ultraclean nanotubes with electrical circuits of arbitrary complexity is still a challenge. We develop a new directly deterministic placement technique that allows us to operate each CNT under an optical microscope and ambient conditions. For an individual ultralong few walled CNT, After deposit TiO₂ nanoparticles on the suspended part of it for visualization, we draw the inner shell of the CNT, and transfer it between the two homemade tips, then place it to the target placement on the device chip. The CNTs transferred by this method are perfect clean since they are inner shell of the CNTs and not suffer from any wet process. The way to transfer and placement is so flexible and steerable that the construction of complex multi-nanotube devices can be allowed. Use this technique, we fabricate the CNT electromechanical resonators and achieve the strongly nonlocal coupling of the phonon modes between neighboring resonators.

B16: Bolometers on hybrid films based on SWCNTs and graphene

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Optical detectors become more and more important in modern industry. With the development of different technologies new devices for the detection of different

radiation ranges appear. Here, we report fabrication of infrared detectors (bolometers) based on free-standing single-walled carbon nanotube (SWCNT) films. To optimize the characteristics of bolometers in terms of response time, wavelength sensitivity and noise equivalent power (NEP), we have varied the properties of produced SWCNTs to adjust the properties and created the hybrid material SWCNT/graphene. We have built the first prototype of the device, which is comparable with similar products on the market. The optimized structure of the bolometer demonstrated excellent performance. A major advantage of our solution is the ease of implementation into production, the ability to create arrays on the basis of a single cell, and unlimited possibilities for the miniaturization of the system. This research was supported by the Ministry of Education and Science of Russian Federation under the grant agreement no. 1425320 (Project DOI: RFMEFI58114X0006).

B17: Carbon nanotube fibers for wearable devices and smart textiles

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With the rapid development of wearable electronics, scalable fabrication of flexible electronic fibers is of great significance for integrating functional components into textiles and providing accesses to generate and store energy, sense and response to environmental stimuli, and communicate with human body . Recently, tremendous efforts have been made on developing coated energy textiles, fibrous devices and device knitting. Among various fibers used for wearable electronic devices, carbon nanotube (CNT) fiber has demonstrated superior advantages such as superior mechanical strength and modulus, extraordinary flexibility, high thermal and electrical conductivities, and novel resistivity to corrosion and oxidation . In this talk, I will summarize our recent research on the scalable preparation of CNT fibers, structural modification for mechanical and electrical enhancement of CNT fibers and their applications in flexible and wearable devices for energy harvesting and storage, and sensing.

B18: Carbon nanotube field-effect transistors based medium scale integrated circuits with single and low supply

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Carbon nanotubes are believed to be a promising channel material in constructing integrated circuits. Recent years CNT circuits have been vigorously developed. But CNT circuits are still limited in conducting simple function, and suffer from low yield,

poor output voltage level, relative high working voltage and need for multiple feed. Here we present a systematic work from transistors to integrated circuits based on carbon nanotube networks. High uniformity and 100% yield p-type CNT transistors were batch fabricated with yttrium oxide as gate dielectric and palladium as contact. Inverters with gain ~ 100 ($V_{DD}=2V$) and 83-stage ring oscillator (166 transistors) were achieved. CNT circuits made from these transistors have the merit of almost rail-to-rail output, relative low working voltage ($V_{DD}=2V$) and single power supply. High performance circuit unit such as NAND, AND, NOR, OR, XOR, XNOR, d-latch and shifter were made as building blocks for integrated circuits. A full-adder was fabricated and based on it a four-bit adder of medium scale integration was achieved. Besides, a carbon nanotube multiplier was first realized, performing full function of 2-bit multiplication. These achievements indicate the capability of CNT circuits to conduct more complex operation.

B19: Contacts dominated room temperature broadband infrared cascading detector based on carbon nanotube with high responsivity, detectivity and stability

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Infrared (IR) detectors are important for a variety of industrial and scientific applications such as IR imaging, biological sensing, day and night surveillance and communication¹. However, most high-end IR detectors made of conventional semiconductors need to be cooled to achieve high performance, and these materials are usually not stable under strong illumination. Carbon nanotubes (CNTs) are direct-bandgap materials with broad spectral response and large absorption coefficient². Existing CNT based IR detectors, however, either require bias to operate or are based on individual CNTs with limited absorption and thus performance³. Here, we show that contacts dominated high performance photodiodes or IR detectors can be constructed based on high-purity solution-processed CNTs via a doping-free technique, which can further be combined with virtual contacts to multiply photovoltage and thus to improve the signal to noise ratio. Using photovoltage as the signal, it is shown that the CNT film based IR detector has a broadband response from 1200 nm to 2100 nm, high room temperature responsivity and detectivity of up to 1.5×10^8 V/W and 2.91×10^{11} Jones separately, which can be compared with state-of-the-art InGaAs detectors¹, and extremely good temperature and temporal stability. Large scale fabrication potential is also demonstrated by fabricating a 150×150 photodetector array on a two inch wafer. Electric and optoelectronic tests on randomly selected 72 detectors reveal excellent device performance uniformity with a yield of 100%.

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B20: Controlling the interaction of coordination compounds-filled SWCNTs with reactive NO₂

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Controlling the interaction between gases and Single-Wall Carbon Nanotubes (SWCNTs) is a key point for sensors made with nano-carbons [1]. Here we present the latest progress on the understanding of the interaction between nitrogen dioxide and metallicity-sorted ultrapure SWCNTs filled with Ni and Fe [2]. The effect of the different gas dosing on the SWCNTs was measured using UPS, XPS and XAS carried out at SUPERESCA beamline in ELETTRA. The interaction with gas is recognized in the core levels, valence bands and transport measurements. Gas desorption at room temperature was observed, followed by major change in the density of states at the Fermi level. The innovative results help us to get highest selectivity and sensitivity for gas sensing at room temperature. We acknowledge financial support by the FWF, EU.

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B21: Flexible carbon nanotube interdigitated electrode for electrochemical biosensors

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Electrochemical biosensors have attracted much attention because of their potential to realize small-sized point-of-care testing devices. Single-walled carbon nanotube (CNT) thin film is promising material for electrochemical sensors because of its excellent electrochemical properties, i.e., wide potential window, rapid electron transfer kinetics, anti-fouling property and so on. In this work, we have utilized the redox cycle to enhance the sensitivity with an interdigitated electrode (IDE) composed of a CNT thin film. The detection of dopamine (DA) has also been demonstrated with the CNT-IDE. For the electrochemical application of CNT thin films, it is important to realize a CNT thin film with clean surface. Therefore, we employed the dry transfer process to form a CNT thin film [1], in which CNTs were grown by the floating-catalyst CVD, collected on the membrane filter, and then

transferred on a plastic film without contaminations. We also protected the CNT film with SiO₂ from contamination in the sensor fabrication process. The fabricated CNT-IDEs were characterized by four-electrode cyclic voltammetry of K₄[Fe(CN)₆]. The signal current was 14 times higher than conventional planar electrode, showing collection efficiency of higher than 90 %. We also performed the detection of DA, an important neurotransmitter, with the CNT-IDE. The CNT-IDE exhibited good linearity in the detection of DA from 10 nM to 1 μM, covering the DA concentration in blood. Selective detection of DA in ascorbic acid (AA), known as vitamin C, was also demonstrated. The limit of detection of DA was 10 nM in 0.1-mM AA. [1] A. Kaskela *et al.*, *Nano Lett.*, **10**, 4349 (2010)

B22: Impact of tunnel barrier strength on magnetoresistance in carbon nanotubes

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The injection of spin-polarized electrons from ferromagnetic contacts into nonmagnetic materials is a current challenge in the field of spintronics. Carbon nanotubes (CNTs) have excellent properties to study spin transport, as they exhibit ballistic transport, and are expected to have only small spin-orbit coupling and hyperfine interaction, resulting in long spin relaxation and coherence times. Spin injection into two-dimensional graphene is a well-understood phenomenon, however, there was a strong preceding debate about the role of the insulator with regard to spin injection, and ongoing research strives to improve the tunnel barrier even further [1]. Understanding the process of spin injection in its CNTs has proven to be far more difficult, mainly due to two reasons. First, it is difficult to reliably fabricate low-resistive ferromagnetic contacts to CNTs. As a result, a substantial variation of the magnitude of the magnetoresistance (MR) effect between different devices has been observed from early on [2]. Second, the underlying physics of the MR in CNTs is more complex, since the transport regime is determined by the strength of the tunnel coupling between a CNT and the leads. We present a way to compare the MR of different devices from double-wall CNTs with respect to the current regime. We show that this effect is significantly affected by the tunnel barrier strength, which appears to be one reason for the variation between devices previously detected in similar structures. Modeling the data by means of the scattering matrix approach, we find a non-trivial dependence of the magnetoresistance on the barrier strength. Furthermore, analysis of the spin precession observed in a nonlocal Hanle measurement yields a spin lifetime of $t_s = 1.1$ ns, a value comparable with those found in silicon- or graphene-based spin valve devices.

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B23: Induced birefringence in reduced graphene oxide by electric field.

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Graphene can be produced with different methods such as mechanical exfoliation, chemical vapor deposition or chemical method. The latter is interesting for the ease of processability and versatility. This process goes through the formation of an oxidative form of graphene, called graphene oxide (GO), suitable for mass production of graphene by reduction. One of the greatest advantages of GO is its dispersability in water due to the presence of hydrophilic functional groups and, interestingly, GO aqueous suspensions can form liquid crystal phases (LC) above certain threshold concentration. Isotropic GO suspension can also show birefringence by application of small electric fields due to high Kerr coefficient which is very attractive in electro-optical applications [1]. Although reduced graphene oxide (r-GO) is also expected to have discotic lyotropic liquid crystal phases, it is difficult to produce well-dispersed solutions to induce LC phases, especially in aqueous host due to its hydrophobicity. However, reduction in presence of surfactant and selection of mild reductant make it possible to obtain stable r-GO suspension that also exhibits birefringence by shearing and by field. Optical behavior of r-GO under electric field was investigated with measurements of light transmittance between crossed polarizers. R-GO shows superior electro-optical performance and long-term stability compared to GO that can easily degrade at ambient conditions [2].

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[2] M. J. Kim, J. H. Park, J. Yamamoto, Y. S. Kim, and G. Scalia. *Phys. Status. Solidi RRL*, in press (2016). DOI: 10.1002/pssr.201600038

B24: Influence of self-assembled monolayer dielectrics on network density and device performance of SWNT transistors

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Semiconducting single-walled carbon nanotube (s-SWNT) thin films are attractive materials for flexible electronics, *e.g.* in drive transistors of active-matrix displays. It is nowadays possible to separate semiconducting from metallic SWNTs by highly selective polymer-wrapping and thus create SWNT network field-effect transistors (FETs) with high carrier mobilities and high on/off ratios [1]. For the integration of SWNTs in large area electronics uniform and reproducible s-SWNT networks are

required. Further, thin and high capacitance dielectrics are necessary to enable low-voltage operation and short channel FETs. Hybrid dielectrics consisting of a few nm of aluminum oxide (AlO_x) with self-assembled monolayers (SAMs) based on alkyl phosphonic acids are promising for low-voltage, bottom-gate FETs for organic semiconductors [2]. Here, we employ several AlO_x /SAM hybrid dielectrics with different head-groups (imidazolium, amine, hydroxyl and phenyl) and alkyl-chain lengths ($\text{C}_2 - \text{C}_{12}$) in FETs with solution-deposited networks of polyfluorene-wrapped large diameter s-SWNTs. We find a strong impact of the SAM headgroups on the network density for SWNT deposition by dip- and spin-coating. The FETs with gold source-drain electrodes show high on-conductances and good on/off ratios. The device parameters are relatively unaffected by the specific headgroup chemistry, which suggests a screening effect of the polymer wrapping. However, we find a distinct dependence of contact resistance on the SAMs, which limits the critical channel length. Overall, FETs with moderate SWNT coverage on SAMs with long alkyl chains and amine or hydroxyl end-groups showed the best performance with low critical channel length ($< 2 \mu\text{m}$).

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B25: Linear Polarimetry Photodetector and Photoswitch based on Macroscopically Aligned Carbon Nanotubes

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Light polarization is extensively applied in optical detection, industry processing and tele communication. Although aligned carbon nanotube is naturally polarization-related, there is not much work about the research of carbon nanotube's light-wavelength photodetection based on its interaction with polarization. Here, we report a photo-detecting structure with intuitive logic realized by aligned carbon nanotube: due to different absorption of light polarization under changing included angles, the working structure directly responds to specific light wavelength regardless of light intensity. Furtherly, when combined with thermoelectric effect, the corresponding thermoelectric voltage change is also related with specific light wavelength. Theoretical analysis and experiments shows the intrinsic different light absorption of the materials causes the external change of temperatures, which makes aligned carbon nanotube possible to detect specific wavelength. This work may be utilized directly in creating new type of photoswitch, since it can identify a broad spectrum of light from near ultraviolet to intermediate infrared and can be integrated into electric devices easily. A 'wavelength lock' is also demonstrated to explain the feasibility to apply this work.

B26: Nanocarbon-based light sources for integrated optoelectronics and optical communications

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Near-infrared light emitters based on compound semiconductors are widely used in optical communication with optical fibers and silicon photonics. However, because the compound semiconductors cannot be directly grown on silicon wafers, these emitters face significant challenges with respect to their integration with silicon-based platforms. Here we talk about two topics: (i) single photon generation from a carbon nanotubes (CNTs) [1] and (ii) electrically driven, high-speed light emitters based on nanocarbon materials [2-4]. Photon antibunching from semiconductor quantum dots (sQDs) has been attracted much attention for use as single-photon sources in quantum cryptography. However, sQD based single photon sources at both room temperature and telecommunication wavelength have not been reported so far. In this study, we demonstrated the photon antibunching in a SWNT at telecommunication wavelength and room temperature [1]. We also talk about high-speed light emitters based on CNTs and graphene [1-3]. These electrically driven emitters, based on electron-hole recombination or blackbody radiation, have advantages for their integration with silicon-based platforms because of a small footprint and simple fabrication processes, and direct integration on a Si wafer. This work was partially supported by PRESTO and A-STEP from JST, KAKENHI from MEXT, SCOPE from MIC, Core-to-Core from JSPS, Japan.

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B27: Nanomorphology of CNT bundles upon wafer-level fabrication of CNT-FETs

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Dielectrophoretic deposition (DEP) of carbon nanomaterials provides a scalable solution for wafer-level integration of single-wall carbon nanotubes (SWCNTs) yielding field-effect transistors (CNT-FETs) e.g. for high-frequency devices and sensor applications. However, aggregation effect downsizes the performance of the nanoelectronic components. Aside of transmission electron microscopy, there are no methods yet available to analyse the nanomorphology of the CNT superstructures. We address our recent findings on Raman analytics of CNT solids that can be enhanced by depositing gold nanoparticles on the CNT solids. We dispersed semiconducting CNTs of a mixture of chiralities in an aqueous solution of sodium dodecyl sulfate. These CNTs were functionalized with gold nanoparticles as

previously reported. From a detailed Raman analysis of the radial breathing modes we learned that the relative intensity for certain CNT chiralities was selectively affected whereas it remained unchanged for others. This fact allowed us to conclude that the CNT solids are formed from constituents with different diameters and that the aggregate formation energetically prefers a monotonous radial distribution of the CNTs from the outside to the inside. This phenomenon could be observed for CNT fibres generated through DEP alignment as well as for films obtained by drop casting. Based on this finding, we address the possibility to improve the debundling of CNT solids with methods waiving ultracentrifugation. Using a process control by UV-Vis-NIR spectroscopy, our recent work was devoted to bimodal surfactant mixtures. Along a process chain based solely on bath sonication (<80W), tip-sonication (<240 W) and centrifugation (<55000 g) we show that debundling can be improved using a combination of sodium dodecyl sulfate and sodium deoxycholate with respect to the single surfactant.

B28: On-silicon-chip, integrated, high-speed blackbody emitter based on graphene

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High speed light emitters integrated on silicon chips are promising candidate for optoelectronic device in on-chip optical communication. Here, we fabricated graphene based on-silicon-chip light emitter emitting light in near-infrared region exploiting blackbody radiation from Joule heating. In time-resolved measurement, few-layer graphene device demonstrated 1GHz direct modulation of the emission. Moreover, we obtained clear open eye pattern at 1Mbps with multi-layer graphene device. To consider its practical application, we tested durability of the device with graphene capped by alumina under atmosphere and found that the emission did not degrade after 100 hours of measurement. In addition, we also fabricated two dimensional array device to demonstrate high density integration of graphene light emitter using CVD grown graphene. This electrically driven, small footprint and ultra-high speed emitter may open novel applications of blackbody emission such as an integrated light source for integrated photonic or optoelectronic circuit. This work was partially supported by PRESTO and A-STEP from JST, KAKENHI and NIMS Nanofabrication Platform from MEXT, SCOPE from MIC, Core-to-Core from JSPS, Japan. (Contact email: maki@appi.keio.ac.jp)

B29: Photocurrent Spectroscopy of Exciton and Free Particle Optical Transitions in Suspended Carbon Nanotube pn-junctions and Field Effect Transistors

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We report photocurrent (PC) spectra of individual, suspended carbon nanotube pn-junction diodes formed by electrostatic doping using two gate electrodes. Under

various electrostatic doping concentrations, the PC spectra reveal distinctive behaviors for free particle optical transitions and excitonic transitions. In semiconducting nanotubes, the photocurrent generated by excitonic transitions exhibits a strong gate doping dependence, while that of the free particle transitions is gate independent.¹ Here, the built-in potential of the pn-junction is required to separate the strongly bound electron-hole pairs of the excitons, while free particle excitations do not require this field assisted charge separation. We present a detailed model of the built-in fields in these pn-junctions, which, together with phonon-assistant exciton dissociation, predicts photocurrents on the same order of those observed experimentally. Competing photocurrent mechanisms in quasi-metallic nanotubes with bandgaps spanning a wide range from 30 to 180 meV will also be discussed.

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[2] Amer, Chang and Cronin, "Competing Photocurrent Mechanisms in Quasi-Metallic Carbon Nanotube pn Devices" *Small*, 11, 3119 (2015).

B30: Photon antibunching in single-walled carbon nanotubes at telecommunication wavelengths and room temperature

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Single-walled carbon nanotubes (SWNTs), one dimensional materials exhibiting interesting optical properties and unique exciton dynamics, are expected as new single-photon sources in the telecommunication wavelength ranges at room temperature. In this study [1], we measured the photoluminescence and photon-correlation of individual air-suspended SWNTs on a line-and-space patterned silicon substrate from 6 to 300 K over the telecommunication wavelength range. We carried out photon correlation measurements using a Hanbury-Brown-Twiss setup and observed temperature independent moderate antibunching behavior. In order to investigate the exciton dynamics which represent the antibunching behavior, we measured excitation-power and temperature dependence of the photoluminescence spectra and lifetime decay curves. These results indicate that SWNTs are good candidates for single-photon sources operating at room temperature in the telecommunication wavelength range. This work was partially supported by PRESTO and A-STEP from JST, KAKENHI from MEXT, SCOPE from MIC, Core-to-Core from JSPS, Japan. (Contact e-mail: maki@appi.keio.ac.jp)

[1] T. Endo, J. I-Hayase, H. Maki, *Appl. Phys. Lett.*, 106, 113106 (2015).

B31: Printing of aligned carbon nanotube arrays on hybrid dielectric layers for high-performance thin-film transistors

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Semiconducting single-wall carbon nanotubes (SWCNTs), because of their exceptional electronic properties, can be used as active channel materials for the fabrication of high-performance thin-film transistors and logic devices. To realize the full potential of SWCNTs in realistic electronic devices, a scalable approach is highly desired for the simultaneously control their position and orientation. Here, we report a scalable method for the fabrication of aligned carbon nanotubes by printing SWCNT inks on the desired position of organic-modified SiO₂/Si substrates. In this method, the high-purity semiconducting SWCNTs separated by gel chromatography are used as SWCNT electronic inks [1]. The octadecyltrichlorosilane (OTS) molecules were used to functionalize the SiO₂/Si substrate surface. The methyl groups of OTS chains on the SiO₂ substrates exhibiting a strong orientation serve as the ordered template to induce the self-alignment of the printed SWCNTs. Compared to the naked SiO₂ substrates, the fabricated thin-film transistors by printing aligned SWCNTs on the OTS-functionalized SiO₂/Si substrate exhibit much higher performances. The field-effect mobility of devices increase from 120 to 162 cm²/(V s), and on-state conductances increasing from 37 to 55.6 μS and threshold voltage decrease from 6 to 3 V. our present technique is very simple, effective and scalable, which represent an important step in the development of an SWCNT-based electronics device.

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B32: Resonance control of carbon nanotube cantilever on floating potential by electrostatic interaction

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Nanoscale mechanical resonators are widely used for highly sensitive force sensing, where the light weight and high resonance frequency are appropriate for higher sensitivity. Carbon nanotube (CNT) resonators are strong candidates for these applications because of their minute mass and high stiffness. Recently, we have reported oscillation control of CNT mechanical resonator by electrostatic interaction induced retardation, where the electrostatic force was induced by the electron beam irradiation by a scanning electron microscope (SEM).[1] Here, we propose a cantilevered CNT-NEMS on the planar substrate with electrostatic actuation to realize a simple and reliable control of its resonance. For the actuation of the cantilever electrostatically, a pair of Au electrodes is placed underneath the SU-8 support before the fabrication of the CNT cantilever. Note that the resultant cantilevered CNT is electrically floating unlike the conventional electrostatically actuated cantilever, which is directly connected to electrodes. The CNT acts as an

intermediate electrode for a series capacitor between the pair of electrodes. The electrostatic charge induced on the CNT by either DC or AC bias is expected to be the actuation force of the CNT. As a result, the electrical contact resistance between the CNT and electrode is not a matter for device fabrication, which results in the improvement of the device reliability. In the experiment, the AC bias voltage, V_{AC} , was applied between the electrodes for actuation of the CNT resonator. In addition, the DC bias voltage, V_{DC} , was superimposed onto V_{AC} . The amplitude at the resonance is proportional to V_{AC}^2 . Interestingly, the amplitude at resonance also depends on V_{DC} . These behavior can be explained by the simplified series capacitor model with vibrating CNT intermediate electrode.

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B33: Self-oscillation of a carbon nanotube field emitter studied by in situ transmission electron microscopy

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Oscillations of carbon nanotube (CNT) during field emission (FE) have been observed [1], though the origin of the oscillations is not well understood. In order to clarify the mechanism of the oscillations, we investigated the phenomena under various geometrical conditions of CNTs (multi-walled CNTs) using transmission electron microscopy. A hypothetical mechanism for oscillations of nanowire or CNT emitters has been proposed [2]; a CNT bends to an anode by the electrostatic force, and then returns to the opposite direction by the elastic restoring force because of the decreased electrostatic force by FE (i.e., discharge). According to this hypothesis, the initial direction of the CNT is required to be inclined from the surface normal of the anode, and the electric resistance of the CNT itself should be larger than the resistance in FE [3]. FE experiments at various inclination angles of a CNT showed that oscillations were observed without any dependence of the angle, even nearly vertical to the anode surface. Measured electrical resistance of a CNT itself was smaller than that in FE. From these results, we consider that the oscillation mechanism of a CNT during FE in TEM cannot be explained by the idea previously reported.

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B34: Single-wall carbon nanotube/polyimide thin film heater

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Transparent electronics device is one of emerging fields of recent electronic devices. A flexible and semi-transparent heater with quick response is an important component for this application. The flexible heater with transparency would provide visibility for heating process which might be useful for material science for investigation of temperature dependence of micro scale structural change such as phase transition of polymer. Here, we report on a flexible and semi-transparent film heater with quick thermal response using single-wall carbon nanotube film. The structure of film heater was a sandwich structure of polyimide-CNT film-polyimide. First, a base polyimide layer by spin-coating on a Si. Next, CNT film was formed by spray coating method onto polyimide film of base layer at 200 °C, where a single-wall carbon nanotube ink (0.1 wt% in water, WaterSolution Gen 2.3 (KH Chemicals)) was used. Note that the polyimide film was coated with 15-nm-thick SiO₂ layer for hydrophilicity. After that, top coat layer was fabricated by the same process for the formation of the base layer.-, followed by the formation of a pair of Cr/Au (5/30nm thick) electrode. Finally, the free standing polyimide-CNT-polyimide film heater was obtained by exfoliating the film heater from the Si substrate. The resultant thickness of the thinnest film heater was only 1.4µm, which is expected to have low thermal capacity. Sheet resistivity was ~200 W /sq with an optical transmittance of ~70%. The transient response of surface temperature of the heater was measured using thermography in ambient air and vacuum. Temperature of the 1-cm-square heater with ~200 W /sq was quickly raised to 60°C in air and 100°C in vacuum with a time constant less than a second. Thus, we have successfully fabricated the semi-transparent thin film heater of 1.4 m m thickness with rapid thermal response through simple fabrication process.

B35: States of antiferromagnetic molecules detected with a carbon nanotube quantum dot

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Carbon nanotubes (CNTs) have some outstanding properties like their high sensitiveness towards changes in the environment and spindependent conductance. Thus, they are ideal devices to investigate the states of antiferromagnetic molecules via electronic transport experiments on functionalized CNTs. In this work, we present experimental data on quantum transport through CNTs covalently functionalized with antiferromagnetic tetramanganese coordination complexes. The experiments reveal a random telegraph signal (RTS), which is presumably caused by interactions between electron spin and the antiferromagnetic spin system. Furthermore, the statistics of the RTS indicate the relevant time and energy scales for transitions in this regime.

B36: Study of Carbon Nanotubes as Etching Masks and Related Applications in the Surface Modification of GaAs-based Light-Emitting Diodes

Chen, Mo (Department of physics, Tsinghua University, Beijing, CHN)

We report a simple method for nanostructure fabrication using super-aligned multi-walled carbon nanotube (SACNT) thin films to enhance output light power of gallium nitride (GaN) and gallium arsenide (GaAs) based light-emitting diode (LED) devices. The CNT films were used as etching mask for top-down etching process, the morphology of the carbon nanotube (CNT) networks can be transferred to the substrate material. Meanwhile, the CNT films can also played a role as a framework, combined with electron beam evaporation and annealing process, Au nanoparticles arrays can be fabricated on substrate surface. The nanostructures on the tens nanometers scales on the devices surface reduced the internal reflection and lead to the enhancement of light extract efficiency, compared with standard planer device. These processes show no negative influences on the device performance, and should be easy to extend to various research fields and have broad prospects in commercial applications, because of its simple, cheap, and suitable for mass production in the semiconductor industry.

B37: Sub-nanosecond light pulse generation with waveguide-coupled carbon nanotube transducers

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Solution-processed single-walled carbon nanotubes (SWNTs) have recently been scalably integrated into low-loss optical waveguides and operated as electrically-driven light emitters (1,2). The CMOS-compatible framework provides efficient coupling of SWNT-emitted broadband light into nanophotonic circuits. In combination with a nanobeam cavity individual SWNTs transform into narrow-linewidth light sources emitting at arbitrary designed wavelength (3). Such devices with versatile functionalities are of interest for conversion of fast electrical signals into optical ones within a nanophotonic circuit. Here, we demonstrate that waveguide-integrated SWNTs are promising high-speed transducers for light pulse generation in the GHz range with decay times below 80 ps. These results show the potential of SWNTs for hybrid opto-electronic systems and fast, nanoscale on-chip light sources. FP and RK acknowledge funding by the Volkswagen Foundation. RK acknowledges support by Helmholtz society through program STN and the KNMF.

[1] S. Khasminskaya, F. Pyatkov et al., *Adv. Mater.* 26, 3465-3472 (2014).

[2] R. G. Fechner, F. Pyatkov et al., *Opt. Express* 24(2), 966 (2016).

[3] F. Pyatkov et al., accepted by *Nat. Photon.* (2016).

B38: The hydrogen sensor manufacture based on carbon nanotube yarns sheets and Pd thin film

Nahm, Seung Hoon (Korea Research Institute of Standards and Science, Daejeon, KOR); Jeon, Sang Koo (Korea Research Institute of Standards and Science, Daejeon, KOR); Kwon, Oh Heon (Pukyong National University, Busan, KOR); Jang, Hoon Sik (World Tech Co., Ltd., Daejeon, KOR)

Spin-capable multi walled carbon nanotubes (MWCNTs) were grown on the SiO₂ wafer by chemical vapor deposition. The MWCNT sheets were fabricated by being sequentially pulled out from the MWCNTs forest and were carefully deposited on the new SiO₂ wafer. The palladium (Pd) film was deposited on the MWCNT sheets using the sputter and its thickness was 10 nm and finally hydrogen sensor was manufactured. And Au thin film was designed as the electrodes for measuring the resistance change when the hydrogen sensor was exposed into hydrogen. Only Au-electrode MWCNT sheet films show no response to hydrogen gas, whereas Pd coated on the MWCNT sheet films is sensitive to middle concentration hydrogen gas of range from 0.1 to 2 %. Its response value for the relative resistance change increase with an increase in hydrogen concentration. We confirmed that it was appropriate for hydrogen sensor.

Acknowledgement: This work was supported by the National Research Council of Science & Technology (NST) through Creative Agenda Project (CAP-11-5-KRISS)

B39: The voltage generation by movement of electrolyte solution on carbon nanotube thin film

Yasunishi, Tomohiro (Nagoya University, Nagoya, JPN); Kishimoto, Shigeru (Nagoya University, Nagoya, JPN); Ohno, Yutaka (Nagoya University, Nagoya, JPN)

Energy harvesting from environment energy sources is emerging technology for driving IoT sensor devices. Recently, the voltage generation of a few millivolts from the movement of electrolyte solution have been demonstrated by using the graphene [1, 2] and a carbon nanotube (CNT) film [3]. In this work, we investigated the generation induced by the movement of electrolyte solution with highly conductive CNT thin film. The dependence of generated voltage on the CNT film thickness has also been studied. The highly conductive CNT thin films were formed on polyethylenenaphthalate (PEN) substrate by the dry transfer process based on the floating-catalyst chemical vapor deposition. [4]. The size of the CNT thin film was 30 mm x 4 mm. We used 2-mol/l NaCl aqueous solution as the electrolyte. The droplet of the electrolyte solution was moved on the CNT thin film by drawing. We measured voltage or current generated both ends of the CNT film. We first examined the CNT thin film of a thickness of ~40 nm. The open circuit voltage of 220 mV and the short circuit current of 29.3 nA was obtained when the droplet was moved on the CNT thin film. The generated voltage was increased to 2.72 mV by decreasing the CNT film thickness to ~10 nm. This is probably due to the elimination of shunt current flowing through the underlayer CNTs.

B40: Thermoacoustic Transduction in Individual Suspended Carbon Nanotubes

Mason, Blake (The Aerospace Corporation, El Segundo, USA); Chang, Shun-Wen (The University of Southern California, Los Angeles, USA); Chen, Jihan (The University of Southern California, Los Angeles, USA); Cronin, Stephen (The University of Southern California, Los Angeles, USA); Bushmaker, Adam (The Aerospace Corporation, El Segundo, USA)

We report an experimental measurement of the acoustic signal emitted from an individual suspended carbon nanotube (CNT) approximate 2 μm in length, 1 nm in diameter, and 10^{-21} kg in mass [1]. This system represents the smallest thermoacoustic system studied to date. By applying an AC voltage of 1.4 V at 8 kHz to the suspended CNT, we are able to detect the acoustic signal using a commercial microphone and lock-in detection. The acoustic power detected is found to span a range from 0.1 to 2.4 attoWatts or 0.2 to 1 μPa of sound pressure. This corresponds to thermoacoustic efficiencies ranging from 0.007 to 0.6 Pa/W for the seven devices were measured in this study. Here, the small lateral dimensions of these devices cause large heat losses due to thermal conduction, which result in the relatively small observed thermoacoustic efficiencies. The system and results presented here allow us to study thermoacoustic transduction at the single-nanotube level, and better understand the nature of thermal transport at the nanoscale in general.

[1] Mason, B. J., Chang, S.-W., Chen, J., Cronin, S. B. & Bushmaker, A. W. Thermoacoustic Transduction in Individual Suspended Carbon Nanotubes. *ACS Nano* **9**, 5372-5376 (2015).

B41: Three-Dimensional Flexible Complementary Metal-Oxide-Semiconductor Logic Circuits Based on Two-Layer Stacks of Single-Walled Carbon Nanotube Networks

Zhao, Yudan (Tsinghua University, Beijing, CHN)

We have proposed and fabricated stable and repeatable, flexible, single-walled carbon nanotube (SWCNT) thin film transistor (TFT) complementary metal oxide semiconductor (CMOS) integrated circuits based on a three-dimensional (3D) structure. Two layers of SWCNT-TFT devices were stacked, where one layer served as n-type devices and the other one served as p-type devices. Based on this method, it is able to save at least half of the area required to construct an inverter, and make large-scale and high-density integrated CMOS circuits easier to design and manufacture. The 3D flexible CMOS inverter gain can be as high as 40, and the total noise margin is more than 95%. Moreover, the input and output voltage of the inverter are exactly matched for cascading. 3D flexible CMOS NOR, NAND logic gates, and 15-stage ring oscillators were fabricated on PI substrates with high performance as well. Stable electrical properties of these circuits can be obtained with bending radii as small as 3.16 mm, which shows that such a 3D structure is a reliable architecture and suitable for carbon nanotube electrical applications in complex flexible and wearable electronic devices.

B42: Tuning s-SWNT@PFO networks for optoelectronics

Gaufrès, Etienne (Univ. Montpellier, Montpellier, FRA); Gagnon, Philippe (Univ. Montréal, Montréal, CAN); Alvarez, Laurent (Univ. Montpellier, Montpellier, FRA); Paillet, Matthieu (Univ. Montpellier, Montpellier, FRA); Michel, Thierry (Univ. Montpellier, Montpellier, FRA); Zahab, Ahmed (Univ. Montpellier, Montpellier, FRA); Martel, Richard (Univ. Montréal, Montréal, CAN); Izard, Nicolas (Univ. Montpellier, Montpellier, FRA)

The rise of efficient extraction techniques triggered a renewal of interest in semiconducting carbon nanotube (s-SWNT) research. It represents a great interest for optoelectronics, with outstanding properties in field-effect transistor, and s-SWNT ability to efficiently emit light in the near-IR range. In particular, the hybrid system polyfluorene (PFO) wrapped s-SWNT (s-SWNT@PFO) display strong photoluminescence, and could be coupled with photonic devices such as microring resonators to control photoluminescence linewidth and enhance photoluminescence intensity. The main challenge for using s-SWNT@PFO in optoelectronics lies in the difficulty to establish good electrical contact with a PFO embedded carbon nanotube, and existing studies only focused on optical pumping of carbon nanotube networks, without addressing issues of electrical driving. We propose to investigate these issues using suspended s-SWNT@PFO networks. The network formation process allow to control nanotube density, while the amount of remaining metallic nanotube in the network could be adjusted at the extraction phase. A selective annealing process under low pressure is used to tune PFO wrapping around the nanotubes. The resulting s-SWNT@PFO networks are then probed by AFM, Raman spectroscopy, absorption, photoluminescence and electrical experiments.

B43: Ultra-thin Graphene/Polymer Layered Composite Membranes for NEMS applications

Vijayaraghavan, Aravind (University of Manchester, Manchester, GBR); Berger, Christian (University of Manchester, Manchester, GBR)

Single layer chemical vapor deposited (CVD) graphene has shown great promise in enabling Micro and Nano-electromechanical Systems (MEMS/NEMS) that can outperform current silicon-based state of the art. However, current methods in forming single layer graphene electromechanical devices result in low yields due to capillary effects acting on the suspended material during the graphene transfer process. In addition, the suspended membranes that survive often suffer from a distorted topography due to transfer polymer residue thereby limiting the in-plane span as well as poor device fabrications reproducibility. We present the fabrication and mechanical characterisation of a suspended graphene/parylene-C bilayer composite membrane that aims to tackle the prevailing challenge of constructing high yield, environmentally robust suspended devices whilst preserving the superlative mechanical properties of graphene. The fabrication method enables the construction of suspended membrane structures that can be multiplexed over entire wafers with 100% yield. Furthermore, we measure the elastic properties of graphene/parylene-C membranes with different polymer thicknesses ranging from 15nm to 200 nm using a

micro-blister inflation technique. Using this technique we obtain a 2-d elastic modulus of graphene of 173 ± 55 Nm⁻¹ and a bulk elastic modulus of parylene-C of 2.8 ± 0.2 GPa [1] which is consistent with previous reports. The graphene-polymer bilayer structure can be finely tailored to obtain a highly robust mechanical structure that proves to be an excellent candidate for large scale integration in NEMS and MEMS applications [2].

[1] Berger C, Vijayaraghavan A, et al Submitted, 2016

[2] Berger C, Vijayaraghavan A, et al Submitted, 2016

POSTER SESSION C: Toxicology & Biomedical Applications

C1: PIK3CA Amplification Is Common in Left Side-Tubular Adenomas but Uncommon Sessile Serrated Adenomas Exclusively with KRAS Mutation.

Yang, Kiwook (Keimyung university school of medicine, Daegu, KOR)

Colorectal cancer is a heterogeneous disorder than arises via multiple distinct pathways, from tubular adenomas (TAs) and sessile serrated adenomas (SSAs), which are clinically, morphologically, and molecularly different. We examined PIK3CA amplification in colorectal precancerous legions, including TAs and SSAs. DNA was isolated from paired normal and tumoral tissues in 64 TAs and 32 SSAs. PIK3CA amplification, KRAS mutation, and BRAF mutation were analyzed by real-time PCR and pyrosequencing. PIK3CA amplification was found in 25% of TAs and 9.4% of SSAs, respectively. KRAS and BRAF mutations were mutually exclusive in both TAs and SSAs. In TAs, PIK3CA amplification was associated with left side and it was mutually exclusive with KRAS mutation. These results suggest that PIK3CA amplification may be early and important event in colorectal carcinogenesis and may drive the development of left-side TAs independently with KRAS mutation.

Program for Tuesday, August 9th 2016

09:00 - 9:45	Key Note Lecture: Andreas Hirsch <i>Functionalization of Synthetic Carbon Allotropes</i>
09:45 - 10:00	Contributed Talk: Raúl Arenal <i>Atomic Configuration of Heteroatomic and Functionalized Carbon Nanotubes probed via Spatially-Resolved EELS</i>
10:00 - 10:30	Intro Posters D: Katalin Kamarás
10:30 - 12:00	Coffee Break & Poster Session
12:00 - 12:30	Invited Talk: Lukas Novotny <i>Near-field Raman spectroscopy of nanocarbon materials</i>
12:30 - 12:45	Contributed Talk: Dmitry Levshov <i>Optical and phonon properties of index-identified double-walled carbon nanotubes</i>
12:45 - 13:00	Contributed Talk: Andrey Chuvilin <i>Reaction kinetics of bond rotation in graphene</i>
13:00 - 14:15	Lunch
14:15 - 15:00	Key Note Lecture: Hisanori Shinohara <i>Utilizing 1D and 2D Space of Nanotubes and Bilayer Graphene</i>
15:00 - 15:15	Contributed Talk: Un Jeong Kim <i>Large Work Function Modulation of Monolayer MoS₂ by Ambient Gases</i>
15:15 - 15:30	Contributed Talk: Phillip Rohringer <i>Selective Enhancement of Inner Tube Photoluminescence in Filled Double-Walled Carbon Nanotubes</i>
15:30 - 16:00	Intro Posters E/F: Aravind Vijayaraghavan
16:00-17:30	Refreshments /Posters
17:30	Walking Tour

TUESDAY

KN2: Functionalization of Synthetic Carbon Allotropes

Hirsch, Andreas (Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Henkestrasse 42, 91054 Erlangen, Germany)

Chemical functionalization of new C-allotropes is of fundamental interest and opens the door to unprecedented materials applications. In principle, the physical and chemical properties of fullerenes, carbon nanotubes (CNTs) and graphene are related to each other, although their levels of development vary considerably. In order to efficiently explore the reactivity of the less developed CNTs and especially that of graphene it is our goal to provide a unifying approach for the chemistry of all three new carbon allotropes. The fullerenes present the first family of synthetic carbon allotropes. Since their availability in macroscopic quantities numerous investigations with respect to their physical characterization and chemical functionalization have been carried out. CNTs - the second new family of C-allotropes - exhibit at least the same potential for unprecedented applications. Their chemistry, however, is much less developed. Although many protocols for covalent and non-covalent CNT functionalization have been published there are still many fundamental problems to be solved. This includes inter alia the highly selective functionalization of metallic- or semiconducting SWNTs, the high throughput isolation of SWNTs with single helicity, the development of general concepts allowing for tunable doping of individualized tubes with single helicity or least defined transport characteristics (metallic – semiconductive). Finally, the youngest representative in the list of new C-allotropes is graphene and the exploration of its chemistry has just begun to start. So far only investigation on the functionalization of defect rich graphene oxide (GO) but not intact graphene itself have been published. Compared to the various flavours of CNTs (broad variation of helicities, single walled, multi walled) graphene is a much more uniform material. This will facilitate the development of its chemistry considerably. We will present a series of new results of covalent and non-covalent functionalizations of fullerenes, carbon nanotubes and graphene.

CT7: Atomic Configuration of Heteroatomic and Functionalized Carbon Nanotubes probed via Spatially-Resolved EELS

Arenal, Raul (Universidad de Zaragoza, Zaragoza, ESP)

The modification of the atomic configuration of pristine carbon nanotubes (NTs) via the incorporation of heteroatoms (B, N or BN) or via the surface functionalization is a perfect way of control their opto-electronic properties [1-5]. However, it is worth noting that a very detailed analysis of this atomic configuration and concentration of the different species of these heteroatomic/functionalized nanotubes is highly required in order to determine their impact on the electronic/optoelectronic properties of the NTs. In this sense, TEM is an essential tool to perform such studies [1-5]. In particular, spatially-resolved electron energy loss spectroscopy (SR-EELS), developed in an aberration-corrected TEM (having access to a close to 1 angstrom electron probe), is the most powerful technique to achieve these goals. In this communication, we present a detailed study of the atomic configuration of different kinds of heteroatomic (CN_x, B_xC_yN_z) and functionalized single-walled NTs via SR- EELS [4-5]. We have examined the different chemical species present in the NTs, determined their average concentration as well as their spatial distribution within the walls and studied their chemical environment and bonding.

[1] R. Arenal, X. Blase, A. Loiseau, *Advances in Physics* 59, 101 (2010).

[2] P. Ayala, R. Arenal, A. Rubio, A. Loiseau, T. Pichler, *Rev. Mod. Phys.* 82, 1843 (2010).

[3] R. Arenal, K. March, C.P. Ewels, X. Rocquefelte, M. Kociak, A. Loiseau, O. Stéphan, *Nano Lett.* 14, 5509 (2014).

[4] R. Wang, A. Lopez-Bezanilla, A. Masseboeuf, M. Monthieux, R. Arenal, to be submitted.

[5] R. Arenal, L. Alvarez, S. Campidelli, R. Le Parc, J.-L. Bantignies, to be submitted.

[6] The research leading to these results has received funding from the EU under Grants Agreements 312483-ESTEEM2, 604391 Graphene Flagship and Marie Curie 642742 - Enabling Excellence, as well as from the Spanish Ministerio Economía y Competitividad (FIS2013-46159-C3-3-P).

IT3: Near-field Raman spectroscopy of nanocarbon materials

Novotny, Lukas (ETH-Zürich)

We use a laser-irradiated optical antenna to map out phonons and excitons in nanocarbon materials (graphene, carbon nanotubes, carbyne) with a spatial resolution of 10nm. We resolve local defects as well as interactions with the local environment. We observe that defects lead to a band renormalization and to trapping of excitons.

CT8: Optical and phonon properties of index-identified double-walled carbon nanotubes

Levshov, Dmitry (Southern Federal University, Rostov-on-Don, RUS); Tran, Huy Nam (Laboratoire Charles Coulomb, University of Montpellier, Montpellier, FRA); Michel, Thierry (Laboratoire Charles Coulomb, University of Montpellier, Montpellier, FRA); Popov, Valentin (University of Sofia, Faculty of Physics, Sofia, BGR); Blancon, Jean-Christophe (Institut Lumière et Matière, University of Lyon, Villeurbanne, FRA); Arenal, Raul (Instituto de Nanociencia de Aragón, Zaragoza, ESP); Zahab, Ahmed Azmi (Laboratoire Charles Coulomb, University of Montpellier, Montpellier, FRA); Yuzyuk, Yuri (Southern Federal University, Rostov-on-Don, RUS); Sauvajol, Jean-Louis (Laboratoire Charles Coulomb, University of Montpellier, Montpellier, FRA); Paillet, Matthieu (Laboratoire Charles Coulomb, University of Montpellier, Montpellier, FRA)

In this communication, we report on the study of intrinsic Raman features of radial breathing-like modes (RBLM) and tangential modes (G modes), as well as of optical properties of individual, spatially isolated, suspended (environment-free) double-walled carbon nanotubes (DWNTs) by combination of High-resolution electron microscopy, Electron Diffraction, Resonant Raman spectroscopy, Rayleigh spectroscopy and Optical absorption. We demonstrate that these features can only be understood in a coherent way by considering the mechanical and electronic coupling between two concentric layers of the DWNTs. These couplings determine the conditions of observation of the modes in the Raman spectra and affect the frequencies of the RBLM [1,2] and G modes [3,4].

We focus in particular on the dependence of G modes as a function of the structural parameters of index-identified DWNTs with different electronic configurations. We find a clear downshift of the inner-layer G modes with respect to the corresponding G modes in equivalent single-walled nanotubes, when the interlayer distance is larger than the nominal van der Waals distance of about 0.34 nm [3]. This experimental behavior is understood by considering the effects of the relaxation of the layers and the interlayer interaction between the relaxed layers [5], both effects contributing to the negative pressure felt by the inner and outer layers.

[1] D. L. acknowledge financial support of Russian Science Foundation (Grant 15-12-10004)

[2] D. Levshov et al, Nano Lett. 2011. Vol. 11, N11. P. 4800–4804.

[3] D. Levshov et al, J. Nanophotonics. 2016. Vol. 10, N1. P. 012502.

[4] Levshov et al, J. Phys. Chem. C. 2015. Vol. 119, 40. P. 23196–23202.

[5] H.N. Tran, Raman scattering and optical spectroscopies of individual pristine and functionalized carbon nanotubes // PhD, University of Montpellier, 2016.

V. N. Popov, (unpublished results).

CT9: Reaction kinetics of bond rotation in graphene

Chuvilin, Andrey (CIC nanoGUNE Consolider, Donostia -San Sebastian, ESP); Skowron, Stephen (School of Chemistry, University of Nottingham, Nottingham, GBR); Koroteev, Victor (Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, RUS); Baldoni, Matteo (School of Chemistry, University of Nottingham, Nottingham, GBR); Lopatin, Sergei (King Abdulla University of Science & Technology, Thuwal, Makkah, SAU); Zurutuza, Amaia (Graphenea S.A., Donostia -San Sebastian, ESP); Besley, Elena (School of Chemistry, University of Nottingham, Nottingham, GBR)

The raise of nanoscience and nanotechnology and necessity to characterize the structure of individual objects consisting of countable number of atoms determined the shift of structure characterization paradigm from bulk methods like X-ray diffractometry to local high resolution methods like electron microscopy. The similar shift in paradigm is urging now in chemistry - chemical processes defining structure and properties of nanoscale and low dimensional objects often constitute a negligible part of the total volume of the material, and thus their assessment by bulk chemical methods is often impossible. The new concept is provided by the time resolved electron microscopy allowing for direct observation of atomic rearrangements. We have adopted the methodology of macroscopic chemical kinetics for evaluation of atomic rearrangements observed by HRTEM and applied this approach for extracting kinetic characteristics of bond rotation in graphene - the fundamental process defining the mobility of defects. Observation of statistically significant number of events at variable experimental conditions allowed decoupling of radiation induced and thermal reaction pathways and obtaining independent estimations of cross-sections and activation energies for direct and backwards rotations. The cross-sections of direct rotation were found to be in a decent agreement with theoretical estimations. Interestingly the backwards rotation is characterized by very high cross-section exceeding theoretical values by 3-4 orders of magnitude. Moreover the threshold energy determined assuming the knock-on induced process appeared to be smaller than the activation energy for thermally induced pathway, which rules out electron-nucleus collision as the main mechanism of energy transfer from electron beam to the sample. We speculate that the energy is transferred through electron-electron interactions via strong coupling of excited electron states with the phonon modes localised around the defect.

KN3: Utilizing 1D and 2D Space of Nanotubes and Bilayer Graphene

Shinohara, Hisanori; Department of Chemistry & Institute for Advanced Research, Nagoya University, Japan

By putting atoms, molecules, and, even, nanowires of various kind into carbon nanotubes (CNT), one can easily and drastically alter the electronic structures, electron transport and magnetic properties of CNTs, in which charge transfers between encapsulates and CNTs may oftentimes play crucial roles [1]. In some cases, novel one-dimensional (1D) nanowires can be fabricated within carbon nanotubes which are not possible to produce in the conventional bulk conditions [2-5]. A similar thing can be achieved when bilayer graphene is used for “sandwiching” atoms and molecules to fabricate unique nano-materials as well as to observe novel phenomena, but in two dimensional (2D) fashion [6,7]. In this talk, I will discuss some unique and novel properties of 1D and 2D nano-space and its application to syntheses of new materials prepared by nanotubes and bilayer graphene, respectively.

- [1] L.H.G.Tizei et al. Phys.Rev.Lett. 114, 197602 (2015).
- [2] H.E.Lim et al. ACS Nano, 9, 5034 (2015).
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- [4] R.Nakanishi et al. Sci.Rep.3, 1385 (2013).
- [5] Y.Nakanishi et al. Angew.Chem.Int.Ed. 54, 10802 (2015).
- [6] Y.Sasaki et al. Appl.Phys.Express, 5, 065103 (2012).
- [7] Y.Sasaki et al. Chem.Phys.Lett. 650, 107 (2016).

CT10: Large Work Function Modulation of Monolayer MoS₂ by Ambient Gases

Kim, Un Jeong (Samsung Advanced Institute of Technology, Suwon, KOR)

Although two-dimensional monolayer transition metal dichalcogenides reveal numerous unique features that are inaccessible in bulk materials, their intrinsic properties are often obscured by environmental effects. Among them, work function, which is the energy required to extract an electron from a material to vacuum, is one critical parameter in electronic/optoelectronic devices. Here, we report a large work function modulation in MoS₂ via ambient gases. The work function was measured by in situ Kelvin probe technique, further confirmed by ultraviolet photoemission spectroscopy and theoretical calculations. A measured work function of 4.04 eV in vacuum was converted to 4.47 eV with O₂ exposure, which is comparable with a large variation in graphene. The homojunction diode by partially passivating a transistor reveals an ideal junction with an ideality factor of almost one and perfect electrical reversibility. The estimated depletion width obtained from photocurrent mapping was ~200 nm, which is much narrower than bulk semiconductors.

CT11: Selective Enhancement of Inner Tube Photoluminescence in Filled Double-Walled Carbon Nanotubes

Rohringer, Philip (Elektronische Materialeigenschaften, AUT)

A highly selective enhancement of the optical response of the inner tubes of double-walled carbon nanotubes (DWCNTs) has been identified upon transformation of the residual C atoms inside the hollow core to linear carbon chains (LCCs) [1]. Using standardized suspensions, we observed that the photoluminescence (PL) intensity of the inner tubes can be increased manifold, reaching a factor of 6 for tubes with (8,3) chirality. This behavior can be attributed to a local charge transfer from the inner tubes to the LCCs, counterbalancing quenching mechanisms induced by the outer tubes [2]. Furthermore, the length of the carbon chain, which can be tailored by varying the growth temperature of the LCCs and investigated by Raman spectroscopy [3], plays an essential role for this amplification, as well as the DWCNT's diameter, that provides a stable environment for the LCCs. These findings provide a viable pathway to enhance the low PL quantum yield of DWCNTs and proof the capability of inner tubes to exhibit photoluminescence.

[1] P. Rohringer et al., Adv. Funct. Mater 2016, DOI: 10.1002/adfm.201505502

[2] M. Wanko et al., arXiv:1604.00483 [cond-mat.mes-hall].

[3] L. Shi et al., Nat. Mater. 2016, DOI: 10.1038/nmat4617, ALSO POSTER OF LEI SHI

POSTER SESSION D: Characterization & Processing

D1: Angle dependence of optical properties of stacked MoS₂ double layers

Hyangsook, Lee (samsung advanced institute of technology, Suwon, KOR)

Optical behaviors of randomly stacked MoS₂ double layers were systematically investigated as a function of tilt angle. By high resolution transmission microscopy (HRTEM), Moire pattern was varied by the period of 30 degree and the size of the super cell was decreased with the larger tilt angle. Photoluminescence (PL) spectra for the various tilt angle measured at 532nm were observed to be strongly correlated with the tilt angle which is in between that of AA' stacked bulk MoS₂ and monolayer MoS₂. By utilizing the observation, electronic properties of monolayer MoS₂ can be engineered by the selection of tilt angle of bi-layers. Theoretical calculations have been conducted to understand the behavior of PL spectrum change depending on the tilt angle.

D2: Band-like transport in highly crystalline graphene thin films from defective graphene oxide materials

Negishi, Ryota (Osaka University, Suita, JPN); Akabori, Masashi (JAIST, Nomi, JPN); Ito, Takahiro (Nagoya University, Nagoya, JPN); Nakatake, masashi (Aichi Synchrotron Radiation Center, Seto, JPN); Watanabe, Yoshio (Aichi Synchrotron Radiation Center, seto, JPN); Kobayashi, Yoshihiro (Osaka University, Suita, JPN)

Graphene oxide (GO), which is produced by the oxidation of graphite, has attracted great interest in the large-area synthesis of graphene owing to cost-effectiveness and mass production. Since GO has rich oxygen-containing groups, much effort has explored such reduction processes as thermal and chemical reductions [1,2]. However electrical performance of the reduced GO (rGO) films is insufficient, since electrical transport properties of the rGO films are described by variable range hopping model through the localization states [3] because of many defects still remaining in the rGO. In this work, we found that the electrical transport property of the rGO thin-films synthesized from defective GO through thermal treatment in a reactive ethanol environment at high temperature above 1000°C shows a band-like transport with small thermal activation energy ($E_a \sim 10$ meV) that occurs during high carrier mobility (~ 210 cm²/Vs). Electrical and structural analysis using X-ray absorption fine structure, the valence band photo-electron, and Raman spectra indicate that a high temperature process above 1000°C in the ethanol environment leads to an extraordinary expansion of the conjugated π -electron system in rGO due to the efficient restoration of the graphitic structure. We reveal that E_a decreases with the increasing density of states near the Fermi level due to the expansion of the conjugated π -electron system in the rGO. This means that E_a corresponds to the energy gap between the top of the valence band and the bottom of the conduction band. The origin of the band-like transport can be explained by the carriers, which

are more easily excited into the conduction band due to the decreasing energy gap with the expansion of the conjugated π -electron system in the rGO.

[1] G. Eda et al., *Nat. Nanotechnol.*, 3 (2008) 270.

[2] D. Li et al., *Nat. Nanotechnol.*, 3 (2008)105.

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D3: Concentration Dependent Photoluminescence of Single-Wall Carbon Nanotubes is Unsuitable for Evaluation of Chirality Distribution

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Since semiconducting single-wall carbon nanotubes (SWCNTs) show bright photoluminescence (PL) at E11 by exciting at E22, we can use it to know a pair of optical transitions, E11 and E22. Further, the each E11 emission intensity is often used to deduce the abundance of specific species in a chirality mixed SWCNTs. For the reliable estimation, however, chirality dependent quantum efficiency and self-absorption effect should be considered. In order to reveal the PL characteristics of SWCNTs, we investigated the SWCNT concentration dependence of PL intensity in a fixed surfactant concentration. In this study, semiconducting SWCNTs containing several chirality species in 1% sodium cholate (SC) aqueous solution were prepared by gel chromatography. To change the SWCNT concentration, the sample was diluted by adding 1% SC solution. It was confirmed that the absorbance increased linearly with increasing SWCNT concentration for all chiralities. On the other hand, the emission intensity increased nonlinearly with increasing SWCNT concentration in the low concentration region in which the optical absorbance of each chirality is lower than 0.8 for 10 mm of cell length. In this concentration region, the E11 emission wavelength was not changed. In contrast, in the high concentration region where the optical absorbance is higher than 0.8, the emission intensity turned to decrease, and the E11 emission wavelength became longer gradually with increasing concentration. The intensity decrease can be explained by a self-absorption effect, and the emission wavelength shift is probably due to a change of local electric field. Importantly, these concentration effects don't depend on the total SWCNT concentration but depend on each chirality concentration. Since the concentrations of individual chiralities are different in a solution, each experimental PL efficiency is different. As a result, PL intensity cannot be used for determination of chirality distribution for the chirality mixed SWCNT sample. Detailed analysis of chirality dependence of the local environmental effects will be given in the presentation. This work was supported by KAKENHI No. 25220602.

D4: Concentration-Dependent Photoluminescence Characteristic of Single-Wall Carbon Nanotubes

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Semiconducting single-wall carbon nanotubes (SWCNTs) show bright photoluminescence (PL) which can be used for estimating a pair of optical transitions (E₁₁ and E₂₂) of individual (n,m) SWCNTs. In the PL measurement, the emission intensity is also important to deduce the abundance of specific species in a mixture or chirality-sorted sample. However, several issues such as environmental effects, chirality dependent quantum efficiency, and self-absorption effect could affect the quantitative abundance estimation. In order to reveal the PL characteristics of SWCNTs, we investigated SWCNT concentration dependence of PL intensity in a constant surfactant concentration. In this study, roughly chirality selected semiconducting SWCNTs suspended in 1% sodium cholate (SC) solution were prepared by gel chromatography. To change the SWCNT concentration, the sample was diluted by adding 1% SC solution. We confirmed that the optical absorbance increased linearly with increasing SWCNT concentration equally for all chiralities. On the other hand, the emission intensity exhibited an even nonlinear increase with increasing SWCNT concentration in the low concentration region (optical absorbance of each chirality is lower than 0.8 for 10 mm of cell length). At this region, the E₁₁ emission wavelength almost kept the initial value. In the high concentration region (absorbance is higher than 0.8), the emission intensity decreased, and the E₁₁ emission wavelength red-shifted gradually with increasing SWCNT concentration. This intensity change is probably explained by a self-absorption effect. The emission wavelength shift is caused by a change of local electric field. These concentration effects depend on the concentration of each chirality but not on the total SWCNT concentration. Since the concentrations of individual chiralities are different in the chirality mixed SWCNT solution, each experimental PL efficiency is different. As a result, the (n,m) species that gives the most bright PL peak changes depending on the total SWCNT concentration although the chirality distribution is not changed. This work was supported by KAKENHI No. 25220602.

D5: Determining chiral angle from the electronic Fabry-Perot interference pattern

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Connecting low-temperature transport spectroscopy features of a single-wall carbon nanotube with a specific microscopic nanotube structure has been an elusive goal so far. While in Coulomb blockade many aspects of the discrete level spectrum are well-

understood, a closer look leads to a fascinating (and puzzling) world of hard questions. Here, we apply a complementary approach [1] and analyze the Fabry-Perot interference pattern of a carbon nanotube strongly coupled to metallic leads [2]. By tuning a gate voltage over a large range, the trigonal warping of the Dirac cones at large energies can be probed. This, in combination with the valley degree of freedom, leads to a superstructure in the interference pattern, i.e., a secondary interference. Measurements on an ultraclean, long and suspended carbon nanotube device at millikelvin temperatures are complemented with tight binding calculations of the transmission for specific chiralities and analytic modelling. Taking symmetry classes of nanotubes [3,4], but also effects of symmetry breaking at the contacts into account, we show that the crucial parameter for the robust secondary interference pattern is the chiral angle. Consequently, the pattern provides valuable information for determining the structure of a carbon nanotube device.

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D6: Electronic transport in multiwalled carbon nanotubes

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In this work, low temperature transport in multiwalled carbon nanotubes (MWNT) has been studied at different diameters and lengths, within 2 - 10 nm, and 0.3 - 3.5 microns, respectively. In a majority of the samples, semiconductivity showed up as a transport gap in the gate voltage controlled conduction, but metallic MWNTs are found in all diameters. The transport gap is seen to be quantitatively determined by a diameter dependent bandgap, and length dependent localization of charge carriers. The bandgap of semiconducting MWNTs is estimated to be smaller than that extrapolated from the conventional expression applicable to semiconducting single wall carbon nanotubes. Our results constitute the first systematical study on size dependent transport and especially of semiconductivity in MWNTs. These results have significant similarities to the current research on graphene nanoribbons (GRN). As graphene does not intrinsically possess a bandgap, GNRs are fabricated, where a gap is created via quantum confinement due to the narrow width of the channel/nanoribbon. The size of the gap is then roughly in a similar inverse relation with the width, as in the case of the diameter dependence of the MWNT's in our work.

D7: Exchanging Surfactants of Semiconducting Carbon Nanotube Ink by Cross-Flow Filtration for Printed Electronics Application

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Single walled carbon nanotubes (CNT) have great potentialities to become a key material for printed electronics. One of the important issues to utilize CNTs in electronic application is to extract highly pure semiconducting (s-) CNTs. Some extraction techniques were developed and various kinds of surfactants were used. The selective adsorption/desorption with agarose gel (ADG) method uses anionic surfactants, sodium dodecyl sulfate (SDS), sodium cholate, and sodium deoxycholate. We have investigated s-CNT ink properties for high-quality printed thin film transistors (TFTs), and found that anionic surfactants deteriorate the TFT characteristics, while nonionic surfactant such as alcohol ethoxylate (AE) showed good results. Therefore, we have studied exchanging the surfactants by cross-flow filtration. First, we prepared aqueous solution of SDS and AE as dummy ink. The dummy ink was circulated through the inner of the cross-flow filter module and the filtrate came out of the outside of it. Pure water of the amount same as the filtrate was replenished to the ink and the cross-flow filtration was carried out for several tens of hours. The micelles of SDS were smaller than those of AE, and SDS should be selectively included in the filtrate. During filtration, the dummy ink and the filtrates were sampled and the SDS concentration was measured to investigate the filtration conditions. Next, s-CNT ink extracted by the ADG method was filtrated to exchange the surfactants to nonionic AE. The SDS concentrations of the filtrates were examined as a process monitor and the final SDS concentration of the s-CNT ink was estimated to be about 1 micro mol/L. We fabricated printed TFTs using the modified s-CNT ink. They were characterized and it was found that on/off ratio increased and device yield was improved by exchanging the surfactants. This work is based on results obtained from a project supported by the New Energy and Industrial Technology Development Organization (NEDO).

D8: Graphene Oxide Film: Metodology And Properties

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The graphene oxide (GO) has recently become an attractive precursor for making graphene-based materials. GO was synthesized by the modified Hummer's method. The obtained dispersion is used to fabricate thin GO films, with an average thickness of a few micrometers, and large superficial area, ~300 cm² or larger. GO films are two dimensional structures fabricated through a bar-coating/drying method. These films show outstanding mechanical behavior, like high Young's moduli and resistance to fracture, making it a material of interest for engineering application due to their virtues of lightness and multiple functionalities. Tensile tests have proven that the enhancement of the tensile modulus and strength of the GO films arose from

increase the concentration of the solution of GO. Some mechanical properties were measured, and were found a Young's Moduli as high as 5.2 GPa and a last resistance of 52.4 MPa for the most concentrated sample. It's also propose that these method is easily manipulate to create hybrid films for other applications as thermal and conducting papers, and reinforced materials.

D9: In-Situ TEM Observation of Motion of Nanostructures Entrapped in Carbon Nanotube

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Single-walled carbon nanotubes (SWNTs) are promising materials to realize the controllable transport of molecules due to their narrow cylindrical cavities. Time-resolved in-situ transmission electron microscopy (TEM) imaging with an atomic resolution enables direct visualization of molecular motion in SWNTs. The back and forth translations of a carbon capsule, LaC₂ nanocrystal, C₆₀ molecules in SWNTs have been subsequently reported.¹⁻³ However, understanding the driving force and mechanisms of the nanoscale molecular motion is still incomplete and requires substantial further work in order to control and harness it for real-life applications. In this study we follow translational motion of different types of nanoparticles investigated by means of 80 kV time-resolved in-situ TEM in order to deduce the driving force of the motion. Prior to electron beam irradiation, the SWNTs were filled with Fe₃(CO)₁₂ molecules,⁴ which then converted into α -Fe nanoparticles and Fe compounds with amorphous carbon in the lumen of SWNTs. The atomic structures of thus formed nanoparticles were determined by high resolution TEM imaging combined with image simulation. Comparison of the results obtained using a Cs-corrected FEI Titan 80-300, operated at 80 kV, with the measurements for the same material on Cs and Cc-corrected FEI Titan 20-80, operated at 20 to 60 kV indicate electrostatic repulsion due to ionization of the nanoparticles by the electron beam as the most likely force propelling the nanoparticles in their translational motion. References 1, Hiroshi Somada et. al. Nano Lett. 2009, 9, 62-65. 2, Jamie H. Warner et. al. ACS Nano. 2009, 3, 3037-3044. 3, Ke Ran et. al. ACS Nano. 2011, 5, 3367-3372. 4, Thilo Zoberbier et. al. Small. 2016, 12, 1649-1657. Acknowledgment We acknowledge the support of the DFG and the Ministry of Science, Research and the Arts (MWK) of Baden-Wuerttemberg within the frame of the SALVE project, ERC Consolidator Grants and EPSRC for financial support.

D10: Length-Sorted, Large-Diameter, Polyfluorene- Wrapped Semiconducting Single-Walled Carbon Nanotubes for High-Density, Short- Channel Transistors

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Samples of highly enriched semiconducting SWCNTs with average diameters of 1.35 nm have been prepared by combining PODOF polymer wrapping with size-exclusion chromatography.

The purity of the material was determined to be >99.7% from the transfer characteristics of short-channel transistors comprising densely aligned sc-SWCNTs. The transistors have a hole mobility of up to $297 \text{ cm}^2\text{V}^{-1} \text{ s}^{-1}$ and an On/Off ratio as high as 2×10^8 .

D10: Revealing the growth mechanism of inner tubes inside metallocene-filled single-walled carbon nanotubes

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Revealing and understanding the growth mechanism of SWCNTs is the key to the synthesis of nanotubes with required properties. The present study aims at revealing the growth mechanism of inner tubes inside nickelocene- and cobaltocene-filled SWCNTs. By combining in situ annealing and Raman spectroscopy measurements, the monitoring of growth dynamics of nine individual-chirality inner tubes (8,8), (12,3), (13,1), (9,6), (10,4), (11,2), (11,1), (9,3) and (9,2) with the diameters from ~ 0.8 to 1.1 nm has been performed with a time resolution of several minutes. The growth mechanism of inner tubes implies two successive stages of the growth on the carburized and purely metallic catalytic particles, respectively. The stages of the tube growth are characterized by the corresponding growth rates and activation energies. The growth rates at both stages are inversely proportional to the inner tube diameter and are also significantly higher for the Co catalyst. The activation energies of the growth on the carburized Ni and Co catalytic particles decrease monotonically with decreasing the tube diameter, while they show the opposite trend for the purely metallic particles. For both metals, there is no dependence of the activation energies on the chirality of inner tubes.

D11: Simultaneous Observation of Multiple Electronic Raman Scattering in Suspended Metallic Carbon Nanotubes

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Recently, a well-defined electronic Raman scattering (ERS) feature was observed exclusively in metallic SWNTs, and was reported to center at one nearest excitonic transition energy (either M_{ii}^+ or M_{ii}^-) and appear only between the laser line and the G-band.[1] Here, we simultaneously observe multiple ERS features resonantly enhanced at the corresponding excitonic transition energies (both M_{ii}^+ and M_{ii}^-), and located as far as ~ 500 meV away from the excitation laser energy. We obtain a positive Fano factor in the Breit-Wigner-Fano lineshape G- band when ERS is located at the higher Raman shift side of G band. This supports that the G band asymmetry originates from the interference between discrete G band and continuous ERS.[2] The ERS features redshift upon bundling whereas the energy difference between ERS+ and ERS- remains constant. Based on the ERS features, 16 chiralities are assigned with confidence in the d_t range of 0.8-1.6nm, using a commercial micro-Raman spectrometer equipped with only two discrete laser lines (532nm and 633 nm).

D12: Accelerating the development of CNT processing and applications guided by rational and new characterization tools

Hata, Kenji (AIST, Ibaraki, JPN)

Even after 25 years following the elucidation of the carbon nanotube (CNT), only a few mainstream applications have reached the market. For this very purpose, AIST has established the CNT Application Research Center whose primary mission is to support the growth of a CNT industry. Prior to the Center, Prof. Sumio Iijima had been guiding the CNT research in AIST and developed a number of important core technologies, such as Super-growth CVD (water-assisted CVD) and e-Dips CVD, from which various new and promising applications have been demonstrated. Our new strategy to achieve this goal is to develop fundamental CNT processing techniques with the guide of rational and new CNT characterization techniques. Apt examples of the new characterization techniques are using plasmon resonance to measure the length of CNTs and using CPS disc centrifuge to characterize the size of the CNT aggregate dispersions. By adopting these characterization tools to various fundamental CNT fabrication processes, such as drawing fibers or coating films, crucial factors were identified allowing us to answer the very simple question: Can you predict if your CNT dispersion can be spun into a fiber or could be coated into films? In this presentation, I will talk about our strategy and ongoing efforts in the aforementioned direction that we believe would serve as an important route in developing CNT applications.

D13: Accurate electrical conductance measurements of individual carbon nanotubes and fibers

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There is presently no reliable, commonly accepted, standard method for the electrical characterization of carbon nanotubes (CNT) or carbon nanofibers (CNF), although several suggestions have been made [1,2]. The small dimensions as well as the potential influence of mechanical strain and surface contaminations are the main obstacles. Hydrocarbons on the surface of CNT/CNF create an insulating layer which can be evaporated by current annealing or other techniques for reducing the contact resistance [3]. However, as most conductance measurements are done in the relatively low vacuum environment of a scanning electron microscope (SEM) [1,2], there is a high risk of electron beam induced depositions (EBID) creating an amorphous layer around the CNT/CNF, which cannot be removed by heating. Here we discuss our findings from two-probe measurements performed on freestanding nanostructures inside a transmission electron microscope (TEM). The relatively higher vacuum of a TEM, as compared to a SEM, prevents the formation of EBID and further build-up of amorphous carbon after initial current annealing, making it possible to probe the conductivity on different points along the CNT/CNF with a reproducible contact resistance. The TEM also provides accurate determination of the dimensions of the nanostructure, thus providing a much higher accuracy in the estimated resistivity in nanoscale objects.

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D14: Analysis of Water States in SWCNTs by Photoluminescence Spectroscopy

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A single-walled carbon nanotube (SWCNT) shows excellent optical properties and has the outer surface and inner space. We have investigated suspended SWCNTs by photoluminescence (PL) and Raman spectroscopy, and revealed the interaction between SWCNTs and water molecules[1][2]. Since adsorbed and encapsulated water molecules increase the dielectric constant around the SWCNTs, the adsorption and desorption of water molecules on the outer surface and inner space of SWCNTs can be observed as changes of the optical transition energy. Here, we measured PL spectra from suspended SWCNTs with various chiralities, whose length was about 10 μm , controlling temperature and water vapor pressure. For PL spectroscopy, a

Ti:sapphire laser (the excitation wavelength ranges from 700 to 850 nm) were used. PL spectra clearly depended on temperature and water vapor pressure, due to adsorption and desorption of water molecules on the outer surface and inner space. Although the environmental condition dependences were basically understood based on the adsorption and encapsulation of water molecules, some of them suggested that the phase of water in SWCNTs also changed depending on conditions. We will discuss the phase of water depending on the temperature and water vapor pressure, considering the dielectric constant of adsorbed and encapsulated water molecules.

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D15: Anisotropic Spin Relaxation in Graphite Intercalated Compounds

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The phenomena of spin relaxation in nano carbon materials is really interesting. These efforts were highlighted by the possibility of using graphene for spintronics. It is generally accepted that in graphene the spin lifetime should be of the order of 100 ns, which seems to be long enough for applications. However, this theoretical finding has not yet been proven by any experimental results, mainly due to extrinsic scattering effects. Because of this technical difficulty, the graphite intercalated compounds (GIC) are investigated as a model system of graphene, due to many similarities. We prepared Li, K, Rb, Cs doped stage-I, II compounds. The most used method to measure spin relaxation is with electron spin resonance (ESR) spectroscopy. We determined the spin lifetime for the mentioned materials using angular dependent ESR and we found that surprisingly the relaxation is anisotropic. Usual spin relaxation phenomena to describe the relaxation of conducting electrons, the Elliott-Yafet theory does not predict anisotropy. We present a model Hamiltonian, which includes the anisotropic spin relaxation, thus agrees with the phenomena found in GICs. We believe that the result is relevant for the spin relaxation properties of chemically doped or biased graphene.

D17: Characterization Of By-Products Collected From The Chemical Vapor Deposition Synthesis Of Nitrogen-Doped Multiwall Carbon Nanotubes

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One of most used methods to fabricate carbon nanotubes is the chemical vapordeposition (CVD). Multiple variations of this method have been implemented to improve or modify the physical and chemical properties of multiwall carbon nanotubes (MWCNT). The nitrogen precursors and controlled experimental variables in the CVD can produce nitrogen-doped MWCNT (N-MWCNT) with bamboo shape morphology [2,3]. The CVD synthesis is always accompanied by waste products. Characterization and analysis of waste or by-products are regularly unexplored [4]. In this work, we focus on the characterization of residual materials which are derived from the synthesis of N-MWCNT by aerosol assisted CVD using two tubular furnaces at 850 °C. The residual materials were collected from the outside the reactor and from the ketone trap. These two residual materials were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopy and X-ray diffraction. Results revealed that shows that the residual are composed by nitrogen-doped Fe@C core-shell nanoparticles and spider-web materials based on single-walled carbon nanotubes.

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D18: Characterization of Single-walled Carbon Nanotubes by Rayleigh Scattering and Imaging Spectroscopy

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Optical spectroscopy is widely used as non-destructive and contactless characterization method of single-walled carbon nanotube (SWNT) samples. Although light-absorption, Raman scattering and photoluminescence spectroscopy have elucidated various optical properties of SWNTs, Rayleigh scattering spectroscopy [1] attracts much attention. Rayleigh scattering can be measured from both metallic and semi-conducting SWNTs, and even SWNTs located on substrates. Therefore, Rayleigh scattering spectroscopy is suitable for investigation of SWNT samples in various situations. Here, we constructed measurement system in order to perform Rayleigh scattering spectroscopy and imaging spectroscopy. Rayleigh scattering spectra and images were measured from various SWNT samples, such as dispersed SWNTs in surfactant solutions, dry-deposition SWNT thin films [2], and suspended SWNTs in air. For example, Rayleigh scattering spectra with tightly focused excitation laser provided the local information of the tube diameter or chirality of SWNT thin films, while Rayleigh imaging with widely expanded laser elucidated the spatial distribution. We will discuss the advantage of characterization of SWNT samples by using Rayleigh scattering and Rayleigh imaging spectroscopy.

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D19: Chirality-Dependent Surfactant Interactions revealed By Systematic Ultracentrifugal and Aqueous Two-Phase Separations

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The discovery that bile salt surfactants are extraordinarily efficient at solubilizing individual, intact single-wall carbon nanotubes (SWCNTs) in water¹, soon enabled the separation of different SWCNT structures for the first time by density gradient ultracentrifugation (DGU),² and more recently also by aqueous two-phase extraction (ATP).^{3,4} Despite very nice results for a number of small diameter SWCNT chiralities that have been isolated as individual species by DGU and ATP, the underlying mechanisms are not fully understood and the number of variables to be explored and optimized is enormous, preventing a systematic extension to other chiralities. Based on the unique capabilities of optical spectroscopy for characterizing SWCNTs, we present a systematic study of the structure sorting of DGU and ATP. We combine a direct *in situ* optical characterization of the centrifuge tubes after DGU⁵ with systematic surfactant-concentration-dependent ATP separations for different (mixed) surfactants and as such obtain a more detailed understanding of and control over both separation mechanisms. These systematic studies confirm that chirality-dependent surfactant interactions determine the separation order.

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D20: Diameter-dependent Wettability of Carbon Nanotube as Studied by Atomic Force Microscopy

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It is well known that nanometer-scale morphology of a solid surface often affects to the wetting characteristics [1]. It is interesting question how a carbon nanotube (CNT) gets wet by liquid, since its surface is regarded as the highly-curved graphene due to its cylindrical feature with nanometer scale diameter. A theoretical study have suggested that the wettability of CNTs with under 10nm diameters modulates as the diameter decrease [2]. In this study, we experimentally examined the correlation between wettability and curvature of individual CNTs with diameters ranging from 1.4 nm to 23 nm by force measurement based on the Wilhelmy's balance method. The tip of a CNT attached to a cantilevered tip was brought into contact with the liquid surface in an atomic force microscope, and the force curve was recorded. Ionic liquid and water was used for liquid. The tube diameter (d) was measured by transmission

electron microscopy in advance. In the Wilhelmy's method, force applied to the CNT due to wetting (F) can be expressed by $F=\pi d\gamma\cos\theta$, where γ and θ are the surface tension and contact angle, respectively. Since γ and θ are substance-specific at macroscale, $F/\pi d$ ($=\gamma\cos\theta$) should be constant. However, experimental results revealed its diameter-dependent deviation for CNTs with diameter less than 10nm. In the case of ionic liquid, CNTs with $d = 10$ nm to 4.5 nm, measured value $F/\pi d$ decreased as decreasing the diameter. This fact is consistent to the previous theoretical prediction. However, it is also found that CNTs with $d < 4.5$ nm exhibited opposite tendency; $F/\pi d$ increased as decreasing diameter. These findings indicate the curvature affects the wettability of CNTs, and the increase of $F/\pi d$ can be probably explained by taking into account of some factors such as number of CNT layers and kind of liquid.

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D21: Direct measurement of carbon inclusion process in single-walled carbon nanotube growth

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For single-walled carbon nanotube (SWCNT) growth, revealing the mechanistic pathway of reactive species leading to effective nucleation, growth, and termination of the CNTs is an important step forward that can improve catalyst efficiency and even offers the possibility of chirality control of SWCNTs. We have employed an environmental scanning transmission electron microscope (ESTEM), with an aberration corrector, operated at 300 kV to record real-time, atomic-resolution videos (6 frames s⁻¹) of SWCNT growth from a Co-Mo/MgO system in a C₂H₂ gaseous environment at typical synthesis temperatures. We show that the carbon species diffuse into the catalyst particle to form metal carbide and then the carbide decomposes to output carbon species during SWCNT growth. The number of carbon atoms, generated by the decomposition of carbide and incorporated in the growing nanotubes, were obtained by analyzing the structural fluctuation in the particle and measuring the change in length of the tube with time. The fluctuation of carbon content inside the catalyst particle can be directly related to the nanotube growth, which can then be used to calculate rates for reaction steps, such as bulk or surface diffusion of carbon atoms through/over a particle and their incorporation into a nanotube. Experimental results were confirmed by reactive molecular dynamics (RMD) simulations. We also show that the nucleation and growth of SWCNTs occurs on select facets of Co₂C catalyst nanoparticle. A detailed description of our structural analysis approach and quantitative measurements of catalyst carbon content and its relationship to nanotube growth will be presented.

D22: Doping dependent G⁺-Band shifts of small diameter polymer-wrapped semiconducting SWCNTs

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Electrostatic or (electro)-chemical doping has a large influence on the Raman response of all carbon allotropes including single-walled carbon nanotubes (SWCNTs). In particular the frequencies of the G⁺- and 2D-mode of SWCNTs are highly sensitive to electron and hole accumulation. Previous studies on large diameter (>2 nm) nanotubes have shown a consistent shift of the G⁺ mode to higher energies. With the option to purify large amounts of almost monochiral small diameter SWCNTs by polymer wrapping it is now possible to test the doping dependent Raman mode shifts for those nanotubes in electrolyte-gated transistors (EGTs) over a wide charge concentration range and with good spatial resolution in working devices [1,2]. Here we show that semiconducting SWCNTs with small diameters (0.76 – 1.05 nm), namely (6,5), (7,5), (10,5), exhibit an initial G⁺-mode shift to lower energies in contrast to polymer wrapped SWCNTs with large (>1.3 nm) diameters.

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D23: Effective separation of metallic and semiconducting single-wall carbon nanotubes by using binary hydrogels

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Since their discovery, single walled carbon nanotubes (SWNTs) have attracted much attention due to their superior mechanical and electronic properties that have led to their use in various applications. Carbon nanotubes are produced as a complex mixture containing metallic (m-SWNTs) and semiconducting(s-SWNTs) parts, making post-synthesis separation of m- and s-SWNTs nanotubes a challenging process. Recently, gel chromatography method has emerged as an effective technique for obtaining metal–semiconductor separation. In this separation strategy, dispersions of nanotubes in the surfactant sodium dodecyl sulfate (SDS) are passed through a gel matrix which is usually composed of agarose or sephacryl gel beads. Novelty of this research relies on using both of agarose and sephacryl gels for increasing the efficiency of the separation. According to optical absorbance spectra of separated s-SWCNT, small s-SWCNTs are adsorbed to dextran gel beads whereas large s-SWCNTs are adsorbed to agarose gel beads. Considering these properties, our group have developed a novel method. By applying a SWCNTs/SDS dispersion to a column containing dextran, small s-SWCNTs observed to be adsorbed to the gel and collected by changing the eluent. This process was repeated for obtained unbundle

solution until there was no any absorption to the gel. Subsequently, the operation continues with agarose gel beads for absorbing the large s-SWCNTs repeatedly until the end of adsorption process. Consequently, we separated nearly all of the small and large s-SWCNTs and m-SWCNTs that passed through the final column as unbundled solution. By only four repetitions, this method is very simple and low cost that can be used for large-scale with higher throughput from raw SWCNTs separation comparing with previously reported methods in literature.

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D24: Electrical conductivity of fabricated and purified carbon nanotubes wire

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As an application to vehicle wire harnesses or motor coils, Carbon nanotubes (CNTs) wire will be strongly expected to the future lightweight cable materials. The electrical conductivity of CNTs is theoretically estimated to be superior to that of copper. The intrinsic properties of CNTs are yet to be well exercised today. Samples were prepared by the floating catalytic chemical vapor deposition (FCCVD) method, optimized the fabrication of the CNTs, controlled structures of CNTs, and purified with heat and acid treatment. The CNT wire include double-walled CNTs was fabricated. In this research, we report that the conductivity of fabricated CNTs wire depended on the CNT layer numbers.

D25: Electron emission from a graphene edge studied by field emission and field ion microscopy

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Graphene with a finite size has edges by itself, and electronic states at the edges exhibit peculiar properties, e.g., localized states, and spin polarization at zigzag edge. In our previous study on electron emission from graphene edges [1], we have shown that FEM (field emission microscopy) patterns from an open graphene edge show a striped pattern (“lip” pattern), consisting of an array of streaked spots; the direction of striation is perpendicular to the graphene sheet, and each stripe is divided into two wings by a central dark band running parallel to the graphene sheet. In the present study, FEM of aluminum (Al) clusters deposited on graphene emitters and FIM (field ion microscopy) of graphene emitters with clean surface are also studied in order to clarify the origin of the peculiar FEM patterns. FEM of Al clusters and FIM of graphene edge, both of which show atomic resolution, suggest that the lip patterns of FEM reflect the symmetries of π orbitals localized at each atom along the graphene edges (possibly zig-zag edge). The central node (dark line) in the pattern is presumably due to the destructive interference of electron waves emitted from π -orbitals on either side of the graphene plane. However, consideration of only π orbitals is inadequate since unoccupied states are filled by electrons when the

graphene is negatively biased for FE experiment. So, emission from electronic states originating from π^* and σ^* orbitals, like interlayer states in graphite interaction compounds [2], may have to be taken into account.

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D26: Equilibrium dynamics of dispersant molecules on nanotube surface as observed by NMR diffusometry: Lateral diffusion, residence time and competitive adsorption

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One of the most common procedures to suspend and separate carbon nanotubes (CNTs) in water is using non-covalent dispersion methods. This is achieved by the adsorption of amphiphilic molecules (such as surfactants and polymers) on the CNT surface through hydrophobic interactions, and colloidal stabilization by electrostatic and/or steric repulsions provided by the surfactant headgroups. Understanding the equilibrium dynamics established between the nanotubes and the dispersant molecules (e.g. the amount of dispersant adsorbed, the binding strength of the dispersant to the CNT surface or the CNT fraction area covered) are important aspects to design more efficient and smarter CNTs functionalizations. Moreover, these parameters may also play an important role in sorting carbon nanotubes with different chiralities through selective binding. Herein we present a ^1H NMR diffusometry study of the equilibrium dynamics of an aqueous dispersion of Pluronic F127 and SWNT. We were able to quantify the fraction of polymer adsorbed, the residence time and detect the polymer diffusing laterally on the CNT surface.¹ These findings support a nonwrapping state for the polymer on the nanotube surface. Using the same NMR methodology, the competitive adsorption between Bovine Serum Albumin (BSA) and F127 was also evaluated. We could detect a displacement of BSA from the SWNT surface by adding F127 to the system. However, the opposite was not observed, which indicates that F127 binds more strongly to the SWNT surface than BSA.² Similar studies of competitive adsorption between the ionic surfactants (SDBS, SDS, S. Cholate, DTAB, CTAB) and F127 were performed. Different trends upon increasing surfactant concentration were observed.

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D27: Filling-induced shifts of the electronic transitions of SWCNTs from two-dimensional fitting of fluorescence-excitation spectra

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Single-wall carbon nanotubes (SWCNTs) possess unique structure-dependent optical and electronic properties that are extremely sensitive to changes in their local environment.¹⁻³ Previously, we have demonstrated that the electronic transitions of SWCNTs shift when various molecules are encapsulated inside their hollow core.³⁻⁵ Such structure-dependent electronic shifts can be experimentally measured by wavelength-dependent NIR fluorescence-excitation (PLE) spectroscopy. The accurate determination of the chirality-dependent shifts is not straightforward as it is complicated by the presence of overlapping signals from multiple chiralities, each with contributions from both excitonic and band-to-band transitions as well as phonon side bands. Therefore, especially the excitation line shape has not been modeled accurately before. We propose a dedicated empirical model for the emission and excitation spectra, allowing to accurately fit the 2D wavelength-dependent PLE data. *This work has received funding from the ERC under Horizon 2020 (679841: ORDERin1D) and the FWO-Vlaanderen.*

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D28: Green, Scalable, Binderless Fabrication of Single-Wall Carbon Nanotube Nonwoven Fabric Based on an Ancient Japanese Paper Process

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We propose a fabrication method for carbon nanotube (CNT) nonwoven fabrics based on an ancient Japanese papermaking process where paper is made from natural plant fibers. In our method, CNT nonwoven fabrics are made by a scalable process of filtering binder-free, aqueous suspensions of CNTs. The aqueous suspension of single-wall carbon nanotube (SWNT) aggregates enabled smooth filtration through a cellulose filter. The “wet SWNT cakes,” which comprised solely of SWNT and water and obtained after filtration, were press dried to fabricate a SWNT nonwoven fabric. This environmentally friendly process employs water and the raw CNT material alone. Moreover, the scalability of this process was demonstrated by manufacturing a large area (A3, 30x42 cm), thick (40-150 micrometer), self-supporting SWNT nonwoven fabric with a density 0.4 g/cm³, basis weight 0.2 g/m², porosity 63%, and specific surface area 740 m²/g. This thick SWNT nonwoven fabric is anticipated to find application as capacitor electrode materials, functional particle-supported

sheets, and filters. Conventionally, a CNT nonwoven fabric (Buckypaper) has been fabricated from filtration of CNT dispersion, however poses some problems. A binder with water or a large quantity of organic solvent is commonly required to make homogeneous CNT dispersions, and the dispersion process results in shortened, isolated CNTs. Such a homogeneous dispersion of isolated CNTs can be filtered by a fine membrane filter, yet, which is easily blocked, and producing thick films is difficult. We applied aqueous suspensions of loosely entangled aggregates of long, as opposed to isolated and shortened, CNTs. The size of these SWNT aggregates in water ranged a few to 100 micrometer, measured by particle image analyzer. The large size avoided filter clogging and afforded the thick nonwoven fabric. This article is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

D29: Impact of Aerosol-Jet Printing on Quality of Semiconducting Carbon Nanotubes

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Large scale sorting and enrichment of semiconducting single-walled carbon nanotubes (s-SWNT) by e.g. selective dispersion with conjugated polymers enables the application of new deposition methods for electronic devices. While spin- or dip-coating in combination with top-down patterning is feasible and gives good results, the waste of s-SWNT material and limited sample sizes are rather disadvantageous. These problems can be overcome with additive techniques, such as gravure, inkjet and aerosol-jet printing. It is still unclear, which of these techniques results in the best device performances, e.g. for field-effect transistors with printed s-SWNT layers, for a given type and amount of carbon nanotubes to be formulated into a printable ink. Although various printed s-SWNT circuits were reported, there are no studies on the influence of the printing process on the deposited material and final device performance. Here, we apply aerosol-jet printing to deposit polymer-sorted (6,5) nanotubes from toluene based inks. Besides finding an optimized ink formulation and process parameters such as temperatures, flow rates, and sonication strength, we analyze the changes of s-SWNT and ink quality caused by the creation of an aerosol via ultrasonication and shear stress during the printing process. The nanotube quality (length, defect-density etc.) is accessed by a number of different techniques such as Raman, absorption and fluorescence spectroscopy as well as atomic force microscopy. Furthermore, we determine the field-effect transistor performance (on-conductance, carrier mobility, hysteresis) of the aerosol-jet printed (6,5) carbon nanotube networks over long printing periods.

D30: In-situ imaging of nanoparticle deposition on SWCNTs using Rayleigh Imaging Microscopy

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Deposition of different nanoparticles on carbon nanotubes is very interesting and has important applications. However, the dynamic of nanoparticle deposition demands studying systematically. The true color real time imaging of single-walled carbon nanotube has been realized by Rayleigh Imaging Microscope. Besides, the Rayleigh scattering of carbon nanotubes can be enhanced by the interface dipole enhancement effect which can be contributed by the interface nanoparticles. Thus, the in-situ characterization of the nanoparticle deposition process can be realized by the Rayleigh Imaging Microscopy. Here, taking advantage of the Rayleigh Imaging Microscope, the whole process of the nanoparticle deposition on single-walled carbon nanotubes is recorded.

D31: Interaction of Polymers with Single-Wall Carbon Nanotubes

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Polymers are widely used for post synthesis processing, purification and individualization of single-wall carbon nanotubes (SWNTs) in aqueous or organic solvent environments. Here, the interaction of single-stranded DNA oligomers (ssDNA) and of a polyfluorene copolymer (F8T2) with (6,5) SWNTs was investigated from desorption kinetics and in the case of ssDNA also using adsorption isotherms. Eyring analysis of desorption rate constants reveals a linear increase of activation enthalpies with ssDNA oligomer length until the desorption enthalpy saturates at $(155 \pm 5) \text{ kJ} \cdot \text{mol}^{-1}$ for oligomers exceeding the ssDNA Kuhn length of about 6 nm. The Gibbs energy for desorption of $(96 \pm 1) \text{ kJ} \cdot \text{mol}^{-1}$ is length-independent due to entropy-enthalpy compensation. The saturation of desorption energies at the high polymer coverages studied here is attributed to incomplete adsorption with typically no more than a single Kuhn segment of a polymer attached to a SWNT.

D32: Local Thermometry for Carbon Nanotubes and Substrates

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Since their discovery, carbon nanotubes (CNTs) have fascinated many researchers due to their unprecedented electrical, optical, thermal, and mechanical properties. We present a simple, rapid and non-invasive technique that enables both optical imaging¹ and local thermometry of CNTs. CNTs serve as a seed for nucleation and growth of small size, optically visible nano-crystals. The nano-crystals sublimation time is used to determine local temperature of CNT/Graphene/other materials. When the nano-crystals completely sublime off the CNT surface, the CNT electrical and mechanical original properties are preserved. This technique allows high lateral

resolution for optical imaging (~250 nm) and enables local thermometry with similar spatial resolution. Our results show a clear distinction of sublimation time between CNTs, heated to different temperatures: 60 +/-5 sec, 142 +/-14 sec and 378 +/-52 sec for 80, 70 and 60 degrees Celsius respectively. This technique will allow future research of direct, in-situ thermometry for CNT-based devices as well as local thermometry for different substrates, both of which can be used to improve heat dissipation engineering techniques for electronic devices.

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D33: Mass production and advanced multi-properties of aligned carbon nanotube fibers, yarns and thin films

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We investigate comprehensively the effects of synthesis conditions and post-treatment processes on the structures and multifunctional properties of the continuous carbon nanotube (CNT) fibers and films that synthesized via a floating-catalyst technique. The production rate of the aligned CNT fibers and thin films is approx. 1.0 km/30 min. A two-step post treatment technique involved acidification and epoxy infiltration is applied to enhance the mechanical and physical properties. The tensile strength and Young's modulus of CNT fibers can increase remarkably by 177% and 325% respectively, while their electrical conductivity also reaches 8,235 S/cm. A simple but effective mechanical densification method is applied on the CNT fibers to produce highly dense CNT ribbons having the electrical conductivity of 12,000 S/cm. After being infiltrated with epoxy on the CNT ribbons, the tensile strength and stiffness of the cross-linked CNT ribbons can reach up to 5.2 GPa and 444 GPa, respectively. Besides, the strength of CNT yarn that is twisted five CNT fibers can approach 3.7 GPa. For the aligned CNT thin films, the as-prepared CNT thin films without acidification exhibit tensile strength and Young's modulus can obtain 400 MPa and 3.09 GPa, respectively; while their electrical and thermal conductivities are 2,200 S/cm and 80 W/(m K). After acid-treatment, the electrical and thermal conductivities can be enhanced to 3,200 S/cm and 400 W/(m K), which is comparable to the thermal conductivity of copper. The acid treatment on CNT is proved to be a promising method for achieving cost effective mass production of high performance CNT fibers, yarns and thin films.

D34: Molecule Assisted Optical Visualization of Carbon Nano-tubes [1]

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Since their discovery carbon nanotubes (CNTs) have fascinated many researchers due to their unprecedented electrical, optical, thermal, and mechanical properties. CNTs have found a wide range of applications in nanoelectronics, composite materials, energy conversion, and sensors. However, a major drawback in utilizing CNTs for practical applications is the difficulty in positioning or growing them at specific locations or in locating them on the substrate such that a circuit can be built around them. We present a simple, rapid, non-invasive, and scalable technique that enables optical imaging of CNTs. We use the CNT as a scaffold for nucleation and growth of small size, optically visible nanocrystals, and image the decorated CNTs by using dark field optical microscopy. The choice of the right molecules for the process allows complete removal of the marking nanocrystals with preservation of the physical properties of the pristine CNT. The high quality and robustness of the new imaging technique allows imaging of 'on surface' CNTs, suspended CNTs as well as van der Waals 2D materials, such as graphene and hexagonal boron nitride. Moreover, we demonstrate that this imaging method allows not only to locate CNTs but also, as in the case of suspended ones, to study their dynamic mechanical motion. The decorated tubes exhibit linear as well as non-linear behavior and for the first time transition from hardening to softening is observed.

[1]. accepted by Nature comm.

D35: Phonon-assisted indirect transitions in angle-resolved photoemission spectra of graphene and graphite

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Angle-resolved photoemission spectroscopy (ARPES) can be used to detect the electron-phonon coupling (EPC) in solids [1]. Most of the previous studies of ARPES in graphene have explored EPC effects on ARPES spectra by the direct observation of the energy bands near the K point. Recently, several ARPES experiments observed the indirect transition of ARPES spectra far from the energy bands around the Γ point and near Fermi energy, where there is no available energy band [2, 3]. In this work, we theoretically investigate the indirect transitions in graphene and graphite by first principle calculation [4], by means of ARPES with several different incident photon energies and light polarizations. Using this technique, the dispersion relation of the transverse optical (TO) and the out-of-plane acoustic (ZA) phonon modes of graphene and graphite can be extracted from the ARPES intensity. We find that the transverse optical phonon mode along Γ -K' and K-M-K' can be observed by

ARPES when the ARPES intensity is explored along the Γ -K with the photon energy about 11 eV using both s- and p-polarized light [5]. The relevant mechanism in this case is the resonant indirect transition. If lower photon energy around 6 eV is applied to the sample, the out-of-plane acoustic phonon mode can be observed through the non-resonant indirect transition with p-polarized light for graphite. Consequently, this technique enables us to unlock the probing of the energy and momentum of the electrons and phonons engaged in EPC from the same measurement via the mapping of the phonon dispersion point that have not been accomplished before.

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D36: Raman Imaging of Long Single-Walled Carbon Nanotubes Grown by Gas-Flow Method

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Growing long single walled carbon nanotubes (SWNTs) is important for practical applications of SWNTs. There are two types of long SWNTs: vertically aligned SWNTs and gas-flow guided SWNTs. Both SWNTs reach to millimeter long, but their densities are quite different. Although the growth mechanism of vertically aligned SWNTs are intensively studied, still little is known about gas-flow guided SWNTs. In this study, we evaluated gas-flow guided SWNTs by Raman imaging and atomic force microscopy (AFM). Raman imaging results showed that the diameters were uniform along the millimeter scale in most cases, different from vertically aligned SWNTs whose diameters increase during growth. Raman images also revealed that each nanotube was not an individual SWNT but a bundle of several SWNTs. This was consistent with the nanotube diameter measured by AFM.

D37: Reliable (n,m) Assignment of metallic SWNTs Based on Multiple Electronic Raman Scattering

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Electronic Raman scattering bands provides a convenient and accurate way to obtain excitonic transition energies M_{ii} of M-SWNTs.^[1] Recently, we observed ERS⁺ and ERS⁻ features simultaneously at the corresponding M_{ii}^+ and M_{ii}^- as far as 500 meV away from laser energy. Here we show (n,m) assignments of suspended M-SWNTs using a commercialized Raman instrument equipped with 532 nm and 633 nm lasers. With these two commonly used laser lines, ERS in the energy range of 1.5-2.3 eV are

observed. More than 16 different chiralities in the d_t range of 0.8-1.6 nm are thus assigned confidently based on ERS and ω_{RBM} . A statistical data on (12,9) chirality shows an almost constant $M_{11^+}-M_{11^-}$ value insensitive to environmental effects, while ω_{RBM} can vary by as large as $\pm 3 \text{ cm}^{-1}$. In addition, an empirical guide to M_{ii} estimation is summarized based on the scattered resonance enhanced phonon Raman spectra, and can be further applied to M-SWNTs in different environments where ERS is not observed.

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D38: Role Of The Acetone In The Growth Of Carbon Nanotube Network

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In the present work carbon nanotube networks (CNT-Net) were synthesized by spray pyrolysis of ferrocene, thiophene, benzylamine, acetone and ethanol at 1020°C employing aerosol assisted chemical vapor deposition using two independent sprayers. The synthesized CNT-Net were characterized by X-ray diffraction (XRD), thermal analysis (TGA), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and Raman spectroscopy (RS). XRD results show that CNT-Net presents turbostratic stacking with interplanar distance of $\sim 3.40 \text{ \AA}$. SEM and TEM characterizations show the presence of well graphitic few layers CNTs surrounded by amorphous carbon layer materials, wavy nanotubes and Y junction structures formed by CNTs. The diameters of the tubular nanostructures are in the range from 40 to 300 nm with metallic nanoparticles average size of 20 nm. TGA results exhibit a loss of weight in the range from 600 to 700°C. This oxidation temperature could be attributed to dangling bonds, interstitial-vacancy defects, and pentagonal-heptagonal membered carbon rings. RS results revealed that D and G bands are found in 1353 and 1595 cm^{-1} , respectively. These resonances correspond to multi-walled carbon nanotubes. Finally, we found that an increment of acetone/ethanol molar ratio increase the yield of CNT-Net.

D39: Selective and reversible non-covalent functionalization of SWNTs by a pH-responsive TTFV-fluorene copolymer

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Single-walled carbon nanotubes (SWNTs) have attracted special attention owing to their extraordinary properties and wide-ranging applications. However, pristine SWNTs exhibit very low solubility in various solvents, making the direct application and processing of SWNTs problematic. To overcome this barrier, non-covalent

functionalization of SWNTs presents a particularly intriguing approach. Although selective interactions between conjugated polymers and SWNTs have allowed isolation of specific SWNT chiralities, the purified SWNTs still retain the conjugated polymer on their surface, leading to low efficiency of SWNT-based devices. To address this issue, strategies for achieving strong and selective interactions between conjugated polymers and SWNTs to produce concentrated dispersions of specific nanotube chiralities, combined with reversible complexation such that the polymer can be desorbed from the nanotube surface upon application of a specific stimulus, are required. In this presentation, I will introduce a new type of tetrathiafulvalene vinyllogous (TTFV)-fluorene copolymer. This copolymer was shown to undergo a conformational change upon protonation with trifluoroacetic acid (TFA). When mixed with single-walled carbon nanotubes (SWNTs), this TTFV-fluorene copolymer exhibited strong interactions with the SWNT surface, leading to stable, concentrated nanotube dispersions in toluene. Addition of trifluoroacetic acid (TFA) to the copolymer-SWNT dispersion resulted in a rapid conformational change and desorption of the polymer from the SWNT surface, leading to precipitation of pure SWNTs that were completely free of polymer. Importantly, the nanotubes isolated after dispersion and release by the TTFV-fluorene copolymer were more pure than the original SWNTs that were initially dispersed.

Ref.: Liang, S.; Zhao, Y.; Adronov, A. *J. Am. Chem. Soc.* 2014, 136, 970.

D40: Self-Aligned Hysteresis Free Carbon Nanotube Field-Effect Transistors

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For more than a decade single-wall carbon nanotubes (CNTs) have been considered as realistic alternative for conventional transistors. Substantial efforts were devoted for their precise positioning and growth for functional operations. Others demonstrated various electrical components and entire logic circuits based solely on CNTs. However, hysteresis phenomenon in the transfer characteristics of CNT field effect transistor (FET) impedes the reproducible electrical performance required for successful realization of any commercial electronic circuit. Here we present a hysteresis phenomenon study of four kinds of CNTFETs architectures and report about a fabrication method for the complete elimination of the hysteresis in CNT-FETs¹. Device types I and II (on-surface CNT and suspended CNT, respectively), both gated by the p-doped Si bulk, exhibit substantial hysteresis which increases with scanning range and sweeping time. This hysteresis can be eliminated under high vacuum conditions for type II but it prevails for type I. Device types III and IV are both suspended CNT-FETs which are gated by a local metallic gate which was patterned self-aligned with the source and drain electrodes for type IV. From the different roles which the global and local gates play for the four types of devices we

could learn about the hysteresis mechanism of this system. Interestingly, and most importantly, type IV devices exhibit no hysteresis at all even at ambient conditions, and hence we believe that such hysteresis free FETs architecture will enable the realization of different CNT based electronic devices and sensors.

¹ M. Shlafman *et al*, Applied Physics Letters, 2016 (accepted).

D41: SEM Images of Single-walled Carbon Nanotubes with high resolution and conductivity information

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Scanning electron microscopy (SEM) is widely used to characterize morphology for its nanoscaled resolution. A low accelerating voltage of ~1kV is preferred while taking SEM images for the single-walled carbon nanotubes (SWCNTs) on insulating substrates. High-contrast and low-resolution images can be obtained for the severe positive surface charging induced by the low accelerating voltage. It cannot meet the requirement for the horizontal SWCNT arrays of high density. By using higher accelerating voltage of ~10kV, the charging condition changes, and the resolving ability of the CNTs is increased by ~5 times, from 20/um up to ~100/um. In the meantime, the conductivity type of the SWCNTs can be distinguished from the the SEM images. The metallic CNTs are brighter than the substrate, while the semiconducting CNTs are darker if the parameter is appropriate.

D42: ssDNA Facilitated Chirality Specific Separation of SWCNTs

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Due to their chirality dependant optical and electronic properties, the isolation of single walled carbon nanotubes (SWCNTs) with specific chirality is of great importance to a range of applications including transistors, sensors and photovoltaics. Here we discuss the use of specific ssDNA oligonucleotides for the purification of SWCNTs by chirality using aqueous two phase separation.¹ SWCNTs with (n, m) of $(8, 4)$, $(6, 5)$, $(7, 5)$ were purified and characterised using AFM, Raman, photoluminescence and UV-Vis. Post-processing of the SWCNT-ssDNA hybrids was completed to determine an effective method to remove the ssDNA after separation. It was found that an enzyme (*Exonuclease 1*) could effectively remove the ssDNA, as confirmed by zeta potential, Fluorescence microscopy, XPS and Scanning Auger microscopy. Finally we determined the energy band diagram of the purified SWCNTs using photoluminescence to determine their band gap and photoelectron spectroscopy to determine the Valence band position and work function. These findings are compared to theory and used to predict photovoltaic performance. [1]. G. Ao and M. Zheng, *Current Protocols in Chemical Biology*, 2015, 7, 43-51.

D43: Strong Coupling Regime and Broadband Tunable Emission of (6,5) Carbon Nanotubes Coupled to Plasmonic Crystals

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The optical properties of semiconducting single-walled carbon nanotubes (SWCNTs) depend directly on their chirality. However, it remains challenging to purify large amounts of monochiral samples with a specific chirality, despite efforts towards controlled growth or post-growth sorting. For the use of SWCNTs in actual optoelectronic devices it is also crucial to achieve high emission efficiency as well as controlled directionality for improved collection or detection. Instead of changing the chirality we modify the optical response (e.g. emission wavelength) of thin films of monochiral (6,5) SWCNTs with periodic arrays of gold nanodisks (NDs) and thus transform them into a broadly tunable light source in the 1000-1500 nm range. As confirmed by simulations, the observed tunable and narrow (~20-40 meV) light emission is caused by the significant enhancement of directed emission via the Purcell effect, where the energy position of the new peaks is governed solely by the interdisk distance. Angle-dependent spectroscopic studies reveal that a directional light emission with a divergence of $\sim 1.5^\circ$ is achieved. The emission is polarized despite the fact that the SWCNTs thin film is completely random. For the samples with a higher density of SWCNTs we were able to push plasmon-exciton interactions from the weak to the strong coupling regime with a coupling rate of over 100 meV. Excitons and plasmons in SWCNTs and plasmonic crystals form a new quasi-particle, i.e. plasmon-exciton-polaritons, clearly visible in our experiments even at a room temperature. Further adjustments of the parameters (e.g. SWCNT density and excitation power) may lead to the Bose-Einstein condensation and thus SWCNT polariton lasing

D44: SWCNT growth using ethanol as precursor - an environmental TEM study

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Single-walled carbon nanotube (SWCNT) growth using alcohol as precursor is not new [1–3]. Nevertheless, the selective growth mechanism is still under discussion, as a direct observation of the growth on atomic scale is challenging. We perform *in situ* environmental transmission electron microscopy (ETEM) which allows high spatial resolution under growth conditions of carbon materials [4]. With low-pressured ethanol as precursor, efficient and reproducible growth of SWCNTs from supported Co nanoparticles can be achieved in the ETEM. By following the growth of individual

tubes, growth dynamics and morphology evolution of catalyst particles and nanotubes are investigated.

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D45: Terahertz and optical characterization of CVD graphene and MoS₂ on different substrates

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With the objective toward speed electronic and optoelectronic devices, terahertz time domain spectroscopy (THz-TDS) is a reliable non destructive tool to characterize thin films, based on a coherent detection, using contactless samples that could be as thin as monolayers. Graphene is the most well-studied two-dimensional material, with singular interesting properties for optoelectronics, flexible or transparent electronic devices. But it shows no gap or semiconducting behavior. Other single-layer materials that are semiconducting, like MoS₂, are promising materials as optoelectronic devices. We analyzed by THz-TDS and optical IR, visible and UV spectroscopy, CVD graphene deposited on different substrates: PET, PEN, quartz, glass and silicon, and MoS₂ on sapphire substrate. Flexible substrates like PET and PEN are interesting for applications as flexible electronic devices, including solar cells. From THz-TDS in the range from 0,1 to 2 THz, we can deduce the transmittance, sheet conductivity [1], refractive index and attenuation. From IR, near UV and visible spectroscopy we obtained the transmittance at those frequency ranges. In the increasing research field of 2D materials, Molybdenum disulfide MoS₂ attracted a great interest due to potential applications as thin film transistors [2] or photodetectors. The existence of a direct bandgap in monolayer MoS₂, gives the possibility of performing MoS₂ field-effect transistors. We analyzed CVD obtained MoS₂ deposited on a sapphire substrate, and observed the coherence of both methods, THz-TDS and IR spectroscopy. The advantage of those methods are that we can get significant parameters (from THz-TDS) related to the sample quality without the need of depositing any electrical contacts or sample preparation.

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D46: Transmitted diffraction and imaging of large area graphene with low energy electron beam

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As a great vision, wafer-scale single crystal graphene is an ideal platform for electronic, photonic, mechanical, and other applications. At present, inch-sized single crystal graphene can be synthesized by chemical vapor deposition (CVD), getting closer to the goal of wafer-scale synthesis. However, crystal characterization of such a large domain is still a tedious work. In this report, we demonstrate that the large area graphene can be characterized with an electron beam of relatively low energy. Transmitted electron diffraction and imaging can be easily achieved. Single crystal graphene domains up to several millimeters can be verified via the diffraction and imaging data. The crystal distribution of polycrystalline graphene can also be obtained and the relation between the crystal orientation of graphene and copper substrate was analyzed. Besides for graphene, the electron diffraction has also been used to study large area MoS₂ sample. Monocrystalline and polycrystalline diffraction have been observed and analyzed. The low energy electron beam was used to study adsorption on suspended graphene. A 2×2 0° water adsorption pattern was first observed at room temperature and density functional theory (DFT) calculations indicate that 2D squashed ice is the most possible adsorption structure.

D47: Triplet Exciton Dynamics in Chirality Enriched SWNT Films

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Single-walled carbon nanotubes (SWNT) show high aspect ratio, thermal and chemical stability and charge mobility, and therefore are promising materials to improve charge extraction in organic photovoltaic (OPV) devices. Since typical charge extraction times in OPV devices are in the microsecond range, the interplay of the desired charged states with long-lived neutral states such as triplet excitons becomes important. Triplet excitons have recently been demonstrated on (6,5) SWNT with an optical yield close to 32 %. Here, we present transient absorption dynamics of (6,5) and (7,5) rich SWNT networks on a femtosecond to microsecond time scale. By a global analysis using spectral shapes from a recently published spectroelectrochemical study, we show the presence of an excess photobleach in both samples which can neither be assigned to singlet excitons nor to charged states. We assign this excess photobleach to triplet excitons and show for the first time the occurrence of triplet exciton transfer from the (6,5) to the (7,5) chirality on a 100 ps time scale. By comparing samples of different SWNT density and varying the pump intensity, we discuss the most probable mechanism for triplet exciton generation.

D48: Unravelling the secrets behind the selection of Semiconducting Carbon Nanotubes with the polymer wrapping technique

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Single Walled Carbon Nanotubes (SWNTs) have been extensively studied due their outstanding properties such as high charge mobility along their axis.^[1] In as synthesized SWNTs two-thirds of the tubes are semiconducting and one third are metallic, therefore, the implementation of SWNT for the fabrication of electronic devices such as field effect transistors (FET) is restrained. Methods to separate metallic and semiconducting tubes have been developed. Non-covalent functionalization of SWNTs using π -conjugated polymers is one them.^[2] To date, different conjugated polymers have been used for the selection of semiconducting SWNTs.^[2,3] However, the influence of different polymer backbones on the process is not completely clear. We used the polymer Poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta [2,1-b;3,4 b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)] (PCPDTBT) for the sorting. This polymer shows good dispersion yield for small diameter HiPCO tubes, and large diameter SO tubes. FETs fabricated with networks of s-SWNT:PCPDTBT showed hole mobility up to $30 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. The comparison of PCPDTBT with Poly(9,9-di-n-dodecylfluorenyl-2,7-diyl)(PF-12) and Poly(3-dodecylthiophene-2,5-diyl) (P3DDT) is used to clarify the role of the polymer backbone on the selection process. For small diameter tubes, the polymers containing sulfur in the backbone, namely, P3DDT and PCPDTBT, showed higher dispersion yield. However, this polymer gives rise to SWNTs solutions with shorter photoexcitation lifetime, which is an indication of small bundle formation.^[4] Longer lifetimes, measured for PCPDTBT- and PF12-wrapped SWNTs are an indication of better individualized HiPCO s-SWNTs. For large diameter SO tubes, the bulkier and less flexible backbones of PCPDTBT and PF12 give rise to a higher dispersion yield.

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D49: Using electron diffraction as a means to evaluate Raman spectroscopy for quantification of M- or S-SWNT%

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Recently there is a growing trend of using resonance Raman technique to quantify the population of a specific type of conductivity in a bulk material. In this work, we use electron diffraction as a means to evaluate its validity. Three SWNTs samples with different diameter distributions, including a ferrocene decomposition floating

catalyst chemical vapor deposition (ferrocene-FC-CVD)¹ SWNT sample and a spark-based FC-CVD (spark-FC-CVD)² sample, in addition to a NIST SWNT reference sample (RM8281), have been investigated. Raman spectroscopy study with three excitation wavelengths of 514, 633, and 785nm was performed to quantify the metallic SWNT concentrations (M%) in the samples. To evaluate the Raman results, electron diffraction (ED) technique was used to directly map the chirality distribution. In the ferrocene-FC-CVD sample, M% was estimated over 90% from Raman analysis at 633nm, but 0% at 514nm, while ED analysis gave about 24%. For the spark-FC-CVD sample, the 633nm Raman analysis led to about 55% metallic tubes, but the 514 laser resulted in less than 2% though ED analysis turned out to be 33%. In particular, the Raman assessment of the well-known (6,5)-dominated NIST reference sample at all three wavelengths of 633nm, 514nm and 785nm, however, showed a small minority of (6,5) tubes, due to the weak resonance of the (6,5) tube with any of those lasers.

To conclude, our results prove that the Raman RBM intensities depend largely on the resonant conditions at certain wavelengths, rather than simply on concentrations. Up to the resonance conditions, some majority nanotube species revealed by electron diffraction measurements induce relatively weak, or even missing RBMs, and vice versa. This certainly leads to an uncertainty over Raman spectroscopy for quantitative assessment of metallic tube concentrations calculating from the relative peak intensities.

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D50: Water Adsorption and Desorption Process on SWCNT Surface Studied by Photoluminescence Imaging and Raman Spectroscopy

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Although we have investigated that water molecules adsorb on the surface of single-walled carbon nanotubes (SWCNTs) and they form stable adsorption layer [1], the detailed mechanism of adsorption and desorption process are still not clear. Here, we examined the water adsorption phenomena on the outer surface of SWCNT by PL imaging spectroscopy with controlling the water vapor pressure. The PL images were observed from suspended SWCNTs between a pair of silica pillars, by using a tunable band-pass filter and a 2D allayed detector. In addition, we measured the temperature distribution in the axial direction by Raman spectroscopy. For PL and Raman spectroscopy, Ti:sapphire laser (the excitation wavelength was 785 nm) was used. The length of suspended SWCNTs was longer than 10 μm . PL images showed a spatial distribution of the water adsorption layer on the outer surface of SWCNT during water adsorption and desorption processes, while Raman spectroscopy revealed temperature distribution along the tube axis. We will discuss the water adsorption phenomena on the basis of temperature gradient.

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D51: Photoluminescence quenching in boron-doped single-walled carbon nanotubes

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Single walled carbon nanotubes (SWCNTs) are ideal candidates for biological sensing applications, since they are strong photoluminescence emitters in the optical region where biological tissues are transparent. Furthermore their optical properties are strongly dependent on the environment surrounding them. We are interested in understanding how substitutional dopants can influence these optical properties. The particular case of Boron doped (CBx)- SWCNTs is appealing for these purposes since these structures exhibit improved stability compared to their pristine counterparts. In this study the optical properties of CBx- SWCNTs were analyzed by optical absorption measurements and photoluminescence excitation mapping and weighted against those recorded on pristine material synthesized by the same method and similar catalysts. Our HV-CVD grown CBx-SWCNTs are especially interesting, since they exhibit a uniquely small diameter distribution compared to other pristine CVD grown SWCNTs. For this study our nanotube material was separated by sonication in DOC, followed by density gradient ultracentrifugation to achieve a higher degree of purification. Photoluminescence excitation mapping shows that the photoluminescence in CBx-SWCNTs is quenched compared to pristine SWCNTs. Our results strongly suggest that CBx-SWCNTs are indeed more metallic compared to pristine tubes when we deal with tubes in the same diameter range.

D52: 2D-TEM investigations of CNTs synthesized within vertical-PAA templates for devices applications

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Self-organized templates such as porous anodic alumina (PAA) templates provide several advantages for controlling the nanostructures growth. Due to its well-ordered structure and the confinement imposed by the pores the PAA template offers a promising approach for cost-effective, stable and efficient carbon nanotubes based devices. Here we present a complete 2D analysis based on advanced electron microscopy techniques devoted to the full characterization of both the PAA structure and CNTs grown using dHF-CVD synthesis method. More exactly we combine the FIB preparation technique with advanced TEM characterization techniques such as STEM-EDX and EELS spectroscopy for the assessment of an accurate correlation between the synthesis parameters and the morphological, structural and chemical

characteristics of both the PAA structure and CNTs grown. TEM analysis of different PAA cross-sections, allowed us accessing precise characteristics such as the pore length and their diameter as well as the inter-pore distance. A detailed analysis on the bottom part of the PAA structure helped us evidencing the presence of branches presence when the anodization voltage used for the PAA preparation was changed. For the CNTs, we first examined the impact of the catalyst pretreatment step performed before the CNTs then we investigated the effects of the additional gas phase activation conditions over the synthesized carbon nanostructures caused by varying the hot-filaments power applied during the growth. The results revealed that the pretreatment conditions determine the catalyst distribution at the bottom pores of the PAA membranes, with a strong impact on the CNTs growth within the PAA templates.

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POSTER SESSION E: Nanotube/Graphene Chemistry & Biology & Medicine

E1: A Raman Study Towards the Effective Purification of Boron-doped Single Walled Carbon Nanotubes

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The bonding environment in the carbon nanotube lattice is changed when heteroatoms such as Boron atoms (B) known as “dopant” is incorporated. This dopant affects the bonding environment and induces changes in the intrinsic properties of a single-walled carbon nanotube (SWCNT). Understanding the bonding environment, the dopant distribution of B atoms and the doping levels in the B-doped SWCNTs is particularly important to bring to reality their potential applications. However, the tubes heterogeneity, their bundling, and the presence of catalytic by-products hinder their direct application. We have mastered the production of B-doped SWCNTs using high-vacuum assisted chemical vapor deposition and this work shows our progress regarding their purification processes using several methods followed by a comparative and descriptive analysis of their Raman Spectra. The density gradient ultracentrifugation method was performed in this work as an alternative to the conventional chemical purification treatment. In order to characterize this material, multifrequency Raman spectroscopy has been performed over chemically treated samples and followed by optical absorption studies for the DGU procedure, this analysis was made before and after the purification treatments, which has allowed us to understand the changes in the tube's morphology and their physical properties. Element analysis using X-ray photoelectron spectroscopy (XPS) and Energy Dispersive X-Ray Spectroscopy (EDX) for a bulk overview in Scanning Electron Microscopy have been used. To the best of our knowledge, this study provides the first attempts to scale up the purification process of doped nanotubes as a significant step toward the application stage of this material.

E2: Magnetic molecules arranged in single-wall carbon nanotubes

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Metal-organic molecular magnets are of great interest because of their unique magnetic properties. These arise from interactions between the molecular compounds in the confined nanospace of single-wall carbon nanotubes (SWCNT), forming one-dimensional structures.

We study the magnetic, electronic and structural properties of such molecular chains by means of X-ray/UV Photoemission Spectroscopy (XPS, UPS), X-ray Absorption Spectroscopy (XAS), X-ray magnetic circular dichroism (XMCD), XRD and SQUID.

XRD data analyzed with the Rietveld method suggests that the intermolecular spacing of the chains is dependent on the nanotube diameter. We discuss magnetic ground states, superparamagnetism and possible bulk magnetic ordering of this system as well as the effect of electron doping by potassium intercalation.

Our work provides interesting insight into the properties of 1D molecule chains that would pave the way towards advanced molecule-based magnets. We acknowledge financial support from the Austrian Science Fund (FWF, p27769-N20).

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E3: New Raman Lines in Small-Diameter Ferrocene Fuctionalized DIPS Carbon Nanotubes

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Small and carbon rich molecules are expected to enter into the CNTs and undergo chemical reactions inside. In several recent experiments new Raman lines appear after transformation of the reacted material at high temperatures. Ferrocene was an appropriate filler and new Raman lines were observed. These so called C_n lines are in resonance with red lasers around 2 eV. In a set of new experiments using small diameter DIPS tubes (D ~ 1.3 nm) we found that the reactions definitely perform inside the tubes. This was concluded from a comparison between tubes which were opened or not opened before the filling process, respectively. Only the opened tubes revealed the C_n lines after transformation. In addition, performing detailed studies with other lasers in the spectral range of 2.17 to 2.34 eV new Raman lines were observed at e.g. 1260, 1345, and 1607 cm⁻¹ with a blue shifted resonance as compared to the C_n lines. It is concluded that during the transformation process several new compounds grow inside the tubes. The new Raman lines and also the C_n lines were not observed if the tubes under investigation had a large diameter. Work supported by the Austrian Science Foundation, Project P27769-N20

E4: A novel strategy: self-expansion construction of carbon nanotube aerogels with three-dimensional, ultralight, and hierarchical cellular structure

Luo, Yufeng (Tsinghua University, Beijing, CHN)

Carbon nanotube (CNT) aerogels have widespread applications in many engineering fields because of their 3D microstructure and unique properties. A novel immersion-self expansion-freeze drying method was developed. CNT aerogels were obtained through a spontaneous expansion of the super-aligned CNT films soaked in the piranha solution (H₂SO₄: H₂O₂=7:3) at room temperature. The 3D self-assembled aerogels have ultralight weight (as low as 0.12 mg·cm⁻³), millimeter-macropores with porosity over 99.95%, high surface area of 298 m²·g⁻¹, and hierarchical cellular structure with cell walls of giant CNT membranes. Resulted from these characteristics, CNT aerogels show advantages in the adsorption of organic solvent and the vegetable oil, and the adsorption capacities can reach 1300 times of their own weight.

E5: A One-Step Route to Nanocarbide Processing, Assembly, Application *Shaffer, Milo (Imperial College, London, GBR)*

The reduction of SWCNTs to nanotubide has been used for almost a decade, allowing true individualisation of SWCNTs without introducing damage typical in sonication and oxidation based processing, while enabling a family of subsequent functionalisation reactions. Recently, we have used the reduction of metal salts to produce SWNT-Au nanoparticle hybrids in situ, revealing further details of nanotubide reactivity. However, the synthesis of nanotubide solutions is typically time consuming, often involving solvent exchange. Through the use of sodium naphthalide (NaNp) in N,N-dimethylacetamide (DMAc), raw SWCNTs can be simultaneously reduced and dissolved, accelerating and simplifying the route to high concentration nanotubide solutions, while retaining high yield and SWCNT integrity. This simple route has been shown to be effective for a host of nanocarbon materials including MWCNTs, ultralong SWCNTs, carbon blacks, and graphenes. The optimal absolute charge concentration has been found to correlate consistently and systematically with the efficiency of individualisation, subsequent functionalization, and the properties of subsequent constructs (including surface area and electrical conductivity). Comparative studies allow the response of nanocarbons with different dimensionalities to be assessed to identify the most appropriate form for specific situations. Examples will be given of the use of reductive processing to generate a range of useful constructs, including networked electrodes for supercapacitors and new materials for protein nucleants.

E6: Effect of pH on Stability of Plasma-Treated MWCNT-Water Nanofluids

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Nanofluids (NFs) - engineered dispersions of nanoparticles in host fluids - containing multi-walled carbon nanotubes (MWCNTs) are currently being studied for applications in catalysis, biological sensors, and gas capture to name only a few. Stability of MWCNTs in the host fluid is necessary to preserve all available surfaces for reactions and long term use of the NFs. The choice of functional groups added to the surface of the MWCNTs through plasma treatment allows for a stable dispersion of MWCNTs in aqueous NFs at different pH. MWCNTs are grown by thermal chemical vapor deposition on a stainless steel mesh and form open forests of short tubes amenable to modification of their entire surface. MWCNTs are plasma treated using a capacitively-coupled RF plasma (13.56 MHz) at 35 W in an atmosphere of ammonia, NH₃, and ethylene, C₂H₄, or carbon dioxide, CO₂, and C₂H₄. Surface analysis by X-ray photoelectron spectroscopy has shown that the deposited layer contains ~22 at% of either nitrogen or oxygen. Functional groups such as amines, -NH₂, are present on the NH₃ plasma-treated MWCNTs (N-MWCNT), whereas MWCNTs treated with CO₂ (O-MWCNT) have carboxylic acid groups, -COOH, on their surface. NFs are prepared by dispersing the plasma treated MWCNTs via ultrasonication in reverse osmosis water at the desired pH, therefore allowing for the

protonation or deprotonation of the functional groups. NFs prepared with N-MWCNT at pH 8 and lower are stable at room temperature, where -NH_2 receives a proton to become -NH_3^+ , but at pH 10 and higher, the amine groups remain neutral and the MWCNTs agglomerate. O-MWCNTs form stable NFs at pH 5 and higher where -COOH deprotonates to -COO^- . Moreover, the quantity of charged groups on the surface of N-MWCNTs affects their stability at higher temperature. Boiling NFs with N-MWCNTs at neutral pH caused the N-MWCNTs to agglomerate whereas a NF at pH 3 could be boiled with no visible agglomeration

E7: Electronic and magnetic properties of doped porous nanostructures

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In the interior of porous nanostructures, such as carbon nanotubes (CNTs) and metal-organic frameworks (MOFs), atoms and molecules can be clustered in low dimensions and exhibit unique properties. Our experiments using Raman, UV-Vis, photoemission, SQUID, electron microscopy and magnetotransport measurements elucidate electronic and magnetic interactions at guest-host molecular interfaces that are responsible for their physical properties. We show that encapsulated inside single-wall carbon nanotubes (SWCNTs), iron and nickel clusters behave as stable single-domain magnets exhibiting large coercive fields as the cluster size becomes as small as the exchange length. In MOFs, metal ions are coordinated to form metal arrays and nanovoids. Magnetic transition metal arrays in MOFs are ideal systems in which we study anisotropic magnetic coupling. Metal ions exposed to the interior voids react with infiltrating molecules, leading to MOF's sensing abilities. We show that the MOF's electrical conduction and magnetic ordering temperature can be tuned by doping with TCNQ. This work was supported by the Austrian Science Funds (FWF), project no. P27769-N20.

E8: GO-LIGNIN hybrid materials synthesis and their evaluation as antibacterial materials

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The emerging problem of increasing pathogen bacteria resistance to one or multiple antibiotics has led to intensive searching for novel agents with the ability to prevent bacterial proliferation. Materials with antibacterial properties have been widely used in everyday life, particularly in the protection of health. These materials prevent adhesion and proliferation of microorganisms in different types of surfaces. Nanomaterials as graphene oxide (GO) have shown significant antibacterial activity closely associated with oxygen functionality of its surface, generating oxidative stress and cellular membrane rupture. On the other hand, investigations point lignin (lig) as a compound with antibacterial properties inherent to its phenolic group functionality. This work focuses on the use of both GO and lignin by taking advantage of their properties to obtain an antibacterial synergistic hybrid as an agent to avoid bacterial proliferation without resistance generation. GO was functionalized with lignin by two different pathways: supramolecular and covalent. The first method allows the possibility to obtain the GO-PEGDA-lig and GO-lig hybrid without the necessity of chemical reactions. Conversely, the covalent pathway used PEGDA as a crosslinker between aminated GO and lignin. The obtained hybrid materials were characterized by spectroscopic techniques such as FTIR and Raman, and microscopy techniques as AFM and SEM. Furthermore, CHNS analysis was also performed. The results point out an excess of lignin in the supramolecular and covalent hybrid materials. Moreover, preliminary biological tests established covalent GO-lig 1:5 as an effective antibacterial material against E.coli DH5 α suspension cultivated and re-suspended in 0.8% saline solution in a concentration of 75 $\mu\text{g}/\text{mL}$.

E9: Photoluminescence modulation of single-walled carbon nanotubes based on local-covalent modification using designed molecules

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Near infrared photoluminescence (NIR PL) of semiconducting single-walled carbon nanotubes (SWNTs) is a unique feature based on the Van Hove singularity in the one-dimensional structures. Recently, PL enhancement of the SWNTs has been reported through a very limited amount of chemical modification by oxygen atom doping as well as sp^3 defect doping on the sp^2 networks, in which quantum yield increment and emission wavelength shifts were observed.^{1,2} The local-covalent modified SWNTs (local-m-SWNTs), therefore, are expected as novel optical materials emitting NIR PL because the pristine SWNTs typically show low quantum yields and the inherent PL is dominated by the tube structures classified by chirality. In this study, we report modulation of the chemical modification-induced PL by molecular design of modifiers that allows energy level shifting³ on the doped sites. It reveals that further modification of the doped sites by covalent or noncovalent approach changes the PL of the local-m-SWNTs. As a result, we observe unique wavelength shifting of the NIR PL originated from the designed doped sites. Thus, the present PL modulation

method provides an important feature of the SWNT PL in both fundamentals and applications including optical devices and bio-imaging/sensing.

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E10: Vibrational and Rotational Motions of Li Cation Encapsulated in C₆₀ Fullerene Investigated by THz Spectroscopy

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Li⁺@C₆₀ (C₆₀ fullerene encapsulating Li⁺ ion) is expected to be used as a molecular switch responding to local electric field. In this work, we have investigated [Li⁺@C₆₀](PF₆)⁻ crystal by THz absorption spectroscopy (0.3 - 10 THz, 4 - 390 K), and found that the Li⁺ ion rotates in C₆₀ fullerene even at 150 K. The rotational motion was disappeared below 50 K, where a new vibrational motion of Li⁺ ion appeared. The crossover from rotational to vibrational mode was successfully explained by a simple quantum-mechanical model on Li⁺ ion, taking into account the van der Waals interaction from C₆₀ fullerene and coulombic interaction from PF₆⁻ ion. The lattice vibration (TO phonon mode) of [Li⁺@C₆₀](PF₆)⁻ crystal was also investigated, which blue-shifted with decreasing temperature. By comparing the resonance frequency and the lattice constant of the crystal, temperature-dependent Gruneisen parameter was derived, and the lattice vibration was found to become harmonic at low temperature, which may be induced by the mode crossover of Li⁺ motion.

POSTER SESSION F: Energy & Environmental Applications

F1: Advances in carbon nanotube-silicon solar cells

Tune, Daniel (Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, GER); Flavel, Ben (Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, GER)

Since first reports in 2007, the field of carbon nanotube-silicon solar cells has seen steady increases in performance up to recent records of over 17 % power conversion efficiency under AM1.5G conditions. There have been many reports exploring device structure-property relationships, materials combinations, the effects of doping, antireflection strategies, and more, from a small but growing research community. However, unlike in the case of the related graphene-silicon solar cells, there are still many questions and ambiguities regarding the underlying mechanism of photovoltaic action in the carbon nanotube-silicon system. As well, the field is still very much in the laboratory proof-of-principle stage with many hurdles to be tackled on the path to real-world prototyping. We will present the latest results of our investigations into carbon nanotube-silicon solar cells and our efforts towards addressing the issues in this field.

F2: An efficient electrode for water oxidation: Nickel hydroxide electrocatalyst on a metal-free nitrogen doped carbon nanotube support

Mossegård, Jonatan (Umeå University, Umeå, SWE)

A promising method to produce hydrogen from solar power is to use solar produced electricity to split water in an electrolysis setup. Here we present a study of an efficient electrode for the oxygen evolution reaction (OER), which represents the sluggish side of the water splitting reaction. A hierarchal electrode is synthesized with nitrogen doped carbon nanotubes (NCNTs) as support for the catalytic material; nano-structured nickel hydroxide. The electrodes are synthesized in a bottom-up approach. NCNTs are first grown on a carbon paper (CP) using a chemical vapor deposition technique. The NCNTs are then decorated with catalyst material in a hydrothermal synthesis process. Scanning electron microscopy imaging reveals that the CP fibers are covered with heterogeneous NCNTs and that the NCNTs are in their turn individually coated with a spiky nickel hydroxide structure. The combination of NCNTs grown on the CP fibers makes up an excellent conducting network which can efficiently work as a metal-free current collector under alkaline conditions.

Both as-prepared electrodes and electrodes first treated in an alkaline solution were tested in a three-electrode electrolysis setup, in alkaline conditions (0.1 M KOH). We find that the overpotential for onset of the OER is roughly 0.27 V, which is amongst the best reported values for OER on transition metal oxides. In contradiction to other reports, the data of this work however indicates that aging the catalytic material in an alkaline solution decreased its activity. In addition, Density Functional Theory simulations were performed to bring deeper insight into the OER pathway on the nickel hydroxide surfaces.

F3: Flash evaporation of perovskite by carbon nanotube films

Wei, Haoming (Tsinghua University, Beijing, CHN); ZHAO, XINGYUE (Tsinghua University, Beijing, CHN); WEI, YANG (Tsinghua University, Beijing, CHN); FAN, SHOUSHAN (Tsinghua University, Beijing, CHN); LIN, HONG (Tsinghua University, Beijing, CHN); JIANG, KAILI (Tsinghua University, Beijing, CHN)

A flash evaporation method for the preparation of perovskite films is reported. Super aligned carbon nanotube films heated by laser beam are employed for the vacuum deposition of hybrid organic-inorganic methylammonium lead iodide perovskite thin films, owing to its small heat capacity and fast thermal response ability. The deposition process is tunable, scalable and extremely rapid, allowing for a straightforward preparation of multilayer structures of different organic-inorganic materials.

F4: Single-walled carbon nanotube films as electron-blocking-layer and transparent electrode for solar cells

Maruyama, Shigeo (The University of Tokyo, Tokyo, JPN)

It was found that a film of single-walled carbon nanotubes (SWNTs) can be a dual-functional layer as electron-blocking-layer and transparent electrode through studies of nanotube-silicon heterojunction solar cells [1,2]. We have demonstrated efficient SWNT/Si solar cells using dry-deposited high-quality SWNTs [1] and honeycomb-structured SWNTs [2]. The SWNT/Si solar cells using the dry deposited SWNT film demonstrated the air-stable power conversion efficiency (PCE) of 11.6% before any intentional doping process. With the stable copper oxide based doping the PCE can be more than 13.5 %. Another stable doping technique will be discussed. This dual functionality is also demonstrated for organic and perovskite solar cells. For organic solar cells, the SWNT/MoO_x/PEDOT:PSS layer was demonstrated as a dual functional layer replacing ITO and organic electron-blocking-layer. Using PTB7/PC71BM mixture as active materials, the PCE of 6 % was obtained for glass substrate and 3.9 % on flexible PET substrate [3]. This dual-functional layer was also demonstrated in double-sided illumination perovskite solar cells using SWNT film instead of electron-blocking-layer and gold electrode with over 9 % PCE [4]. Another perovskite solar cell structure using SWNTs instead of ITO is also proposed [5].

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F5: The effect of lanthanide oxides on the methanol electrooxidation performance of Pt/MWCNTs

Chu, Haibin (Inner Mongolia University, Huhhot, CHN)

The exploration of anode catalyst materials with low platinum loading, high catalytic activity and high CO tolerant ability is one the most important issues for the development of direct methanol fuel cell (DMFC). Recently, CeO₂ are found to be an efficient promoter for the Pt/C catalysts towards methanol oxidation with both higher electro-catalytic activity and better stability [1]. However, the poor conductivity of CeO₂ is not benefit for the fast electron transfer on the electrode catalysts, which may lead to the poor performance of the catalysts. We have synthesized doped lanthanide oxides with different compositions, sizes and exposed facets, and combine them with Pt/MWCNTs [2] via different routes. Then the oxygen storage behaviors and variable valences of lanthanide ions are optimized to improve the electro-catalytic activities and CO tolerant abilities of Pt/MWCNTs in methanol oxidation. After the investigation of the relationship between the interface structures of lanthanide oxide-Pt/MWCNTs, the mechanisms about the promotion of the catalytic performance of Pt/MWCNTs by lanthanide oxides will be discussed.

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F6: Binder-free Nano Sulfur - Mesoporous Carbon Nanotube Electrodes for High-Performance Lithium-Sulfur Batteries

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Binder-free nano sulfur-carbon nanotube composite electrodes are fabricated via a solution-based method. Super-aligned carbon nanotube (SACNT) matrix not only avoids self-aggregation and ensures dispersive distribution of the sulfur nano crystal, but also offers three-dimensional continuous electron pathway, enables electrolyte infiltration, confines the sulfur/polysulfides, and accommodates the volume variations of sulfur during cycling. Mesoporous microstructures are introduced to SACNTs through mild oxidation in air to obtain porous carbon nanotubes (PCNTs). Porous structures ensure electrolyte access for fast lithium transport, provide abundant adsorption points for high sulfur loading, and alleviate active material loss via physical adsorption. Meanwhile, high flexibility and sufficient intertube interaction of SACNT are maintained in PCNTs to support a continuous 3D network electrodes. The nano S-PCNT composite electrode displays reversible capacities of 866 mAh/g at 0.1C for sulfur contents of 60 wt%. Even with a high sulfur loading of 70 wt %, the S-PCNT composite electrode maintains capacities of 760 mAh/g after 100 cycles at 0.1C.

F7: Carbon nanotubes decorated with iron nanomaterials as active catalysts for electrolytic hydrogen production

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Among current technologies for hydrogen production as an environmentally friendly fuel, water splitting has been attracted increasing attention. Water electrolysis is also a promising technique to store intermittent electrical energy from renewable resources such as solar and wind energy in the form of H₂ fuel. Electrochemical water-splitting can be divided into two half reactions: the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). Herein, the process of synthesis of carbon nanotubes (CNTs) is modified to grow efficient electrocatalysts for HER and OER. We grow the CNTs by floating catalyst (aerosol) chemical vapor deposition synthesis. However, during the growth of CNTs, the inactive iron nanoparticles from the iron catalyst source of CNTs (regarded as iron impurities in the literature) are encapsulated in the graphitic layers to protect them from oxidation in air. Therefore, carbon-encapsulated iron nanoparticles (CEINs) decorated on CNTs (CEIN/CNT) are synthesized by this method. For HER, single-shell CEINs decorated on single-walled CNTs exhibit a high catalytic activity for HER in acidic media comparable to that of platinum [1]. For OER, the structure of the CEIN/CNT samples is changed to high quality crystalline maghemite (γ -Fe₂O₃) nanoparticles decorated on CNTs (γ -Fe₂O₃/CNT) through a simple electrochemical method. Then, the γ -Fe₂O₃/CNT sample is introduced as a highly active and durable catalytic material for OER in alkaline media [2]. OER is a critical reaction in electrochemical water splitting and rechargeable metal–air batteries to generate and store clean energy.

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F8: Development of Air-stable n-type single-walled carbon nanotubes for thermoelectric conversion application

Fujigaya, Tsuyohiko (Kyushu University, Fukuoka, JPN)

Thermoelectric (TE) conversion is promising strategy to generate electricity especially from heat for microelectronics such as wearable and portable devices, remote sensors and so on due to their light-weight and static mechanics. To fabricate the TE devices, p- and n-type materials are necessary and inorganic semiconductors such as Bi₂Te₃ and PbTe are often used for current development of the TE devices. However, since these materials are toxic, uneasy to fabricate and scarce, development of the substitutive materials are strongly demanded. Among the several candidates including conducting polymers and metal chalcogenide, carbon nanotubes (CNTs)

are emerged as the promising candidate due to their non-toxicity, processability, abundant resources together with the remarkable electric conductivity, large Seebeck coefficient and light weight. In the development of the CNT-based TE devices, instability of the n-type CNT has been a central issue. In this study, we chose 2-(2-methoxyphenyl)-1,3-dimethyl-2,3-dihydro-1H-benzo[d]imidazole (DMBI) as a n-dopant by following reasons, namely, 1) DMBI are stable itself, 2) the cationic form of DMBI after the hydride elimination was also stable and 3) n-doping of SWNT by DMBI was already reported even the air-stability has not been examined yet. As the results, DMBI-doped SWNT film showed thermally stable Seebeck coefficient of ca. -30 mV/K in our measurement temperature range, indicating the successful n-doping of the film. We also monitored the air stability of the Seebeck coefficient of the films. Seebeck coefficient of DMBI-doped SWNT was very stable for at least 60 days at room temperature. Such a remarkable air stability of Seebeck coefficient has not been realized in the other n-dopants such as PEI, NaBH₄ and cobaltcene. We attributed such an air stability to the strong stabilization of n-doped SWNT by the air stable DMBI cation.

F9: Electrochemical Performances of LiCoO₂ Electrodes with Carbon Nanotube Film as Conductive Layer

Yan, Lingjia (Tsinghua University, Beijing, CHN)

Cross-stacked super-aligned carbon nanotube (SACNT) films were introduced into LiCoO₂-Super P conventional electrodes as conductive layer. The strategy is both simple and effective. With less than 0.02 wt% SACNTs, the electrochemical performances of LiCoO₂-Super P electrodes were improved remarkably with content of Super P decreased to 2 wt%. SACNT films form an integrated conductive network on top of the LiCoO₂ cathodes, which can alleviate electrode polarization effectively. LiCoO₂-2 wt% Super P cathodes with 2-layer cross-stacked SACNT film as conductive layer possess superior cycling stability (150.4 mA h g⁻¹ at 0.1C with a capacity fade as low as 0.15% per cycle) and high rate capability (121.6 mA h g⁻¹ at 2C and 177.6% improvement than that without SACNT conductive layer). The LiCoO₂-5 wt% Super P cathodes with SACNT films possess an impressive capability of 139.7 mA h g⁻¹ at 2C and 123.6 mA h g⁻¹ at 5C, which belong to the best data reported so far for commercial LiCoO₂ particles. Moreover, multiple LiCoO₂-Super P cathodes with SACNT films can be stacked together to meet the actual production requirements, and the electrodes show outstanding electrochemical performances. Such strategy holds great potential for large-scale production.

F10: Enhanced Thermoelectric Properties of Single-walled Carbon Nanotubes-Polyelectrolyte Composites

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Thermoelectric (TE) materials based on single-walled carbon nanotubes (SWNTs) are of great interest for the creation of next-generation energy harvesting devices. The

transport properties of SWNTs can be modulated by the introduction of relatively weak external stimuli.[1–3] We have recently reported the TE properties of SWNTs highly dispersed in polyelectrolytes (PEs).[3] The PE composite containing individual SWNTs exhibited the large Seebeck coefficient (α), which is comparable to those of single semiconducting SWNTs.[4] In order to enhance power factor, it is highly desirable to improve the electrical conductivity (σ). Here we study TE properties of SWNT films filled in PEs. σ values increased as the PEs loading level increased to ~5 wt%. PE-filled SWNTs showed a systematic increase in α up to 71 $\mu\text{V}/\text{K}$ from that of raw SWNTs, $\alpha = 42 \mu\text{V}/\text{K}$. Due to simultaneous improvement in electrical conductivity and the Seebeck coefficient, we found 5.7 times larger power factor ($\alpha^2\sigma$, 550 $\mu\text{W}/\text{mK}^2$) compared to raw SWNTs. This enhancement is considered to be associated with the interaction between SWNTs and PEs. For further investigation of the electronic structure of SWNTs in PE composites, we evaluated near-infrared absorption spectra. Relative absorbance derived from metallic SWNTs decreased compared to raw SWNTs. We believe that, due to effective suppression in metal-derived species induced by adsorption of PEs, TE properties were significantly enhanced.

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F11: Fabrication of Supercapacitor Using Xanthan gum Dispersed Double-Walled Carbon Nanotubes

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Double-walled carbon nanotubes (DWCNTs) exhibit high electrical and mechanical properties due to their coaxial structures. Further, because of their nanosized diameter, DWCNTs have attracted lots of attention for electrode material of supercapacitor. However, DWCNTs have strongly bundled structure as well as the hydrophobic nature of their sidewalls, which limit the capacitance of supercapacitor using DWCNTs. To solve this problem, we have chosen Xanthan gum (XG) for dispersion agent of DWCNTs. Because it is reported that XG can be used as dispersion agent, and the supercapacitor using XG electrode exhibited high capacitance in our previous researches. In this study, we have confirmed the dispersion state of the DWCNTs in aqueous solution using optical spectroscopies. Then, DWCNT/XG sample was heat treated and activated using NaOH in order to make XG-based carbon around the DWCNT porous. Finally, we have fabricated a supercapacitor using DWCNT/XG sample and evaluated its capacitance.

F12: High performance micro-supercapacitors with thick carbon nanotube film electrodes on a thin polymer substrate

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Micro-supercapacitors have attracted increasing attention due to their high power density, durability and safety compared to other energy devices. Compared to conventional supercapacitors, miniaturization of the structure and fabricating the components on a substrate (e.g., Si) result in higher power density and quick frequency response owing to reducing the ion traveling length. Recently, our group succeeded in developing high-performance single-walled carbon nanotube (SWCNT) micro-supercapacitors to have high energy and power densities similar to commercially available aluminum electrolytic capacitors, reducing the size to 1,000 times smaller than them at the same time (*Adv. Energy Mater.* **5**, 1500741 (2015)).

However, the drawback of micro-supercapacitors is their relatively small energy capacity because their small volume of electrodes cannot store much amount of ions. For industrialization, thicker electrodes are desirable to increase the energy capacity, resulting in the increased areal energy density. Furthermore, if the components can be fabricated on a thinner substrate, the volumetric energy density for an entire device can be dramatically improved. Also, such thin film micro-supercapacitors are promising candidates as energy sources for flexible/wearable electronics.

Here, we developed a fabrication process of micro-supercapacitors possessing thick film of SWCNT electrodes on a very thin polymer substrate ($< 2 \mu\text{m}$), where electrodes occupied more than 75% of space in the entire device. As a result, compared to conventional CNT/graphene micro-supercapacitors on a Si substrate ($\sim 0.6 \text{ mm}$), energy and power densities can be increased more than 75 fold when considering all device components. The fabrication process proposed here provides thin and lightweight energy devices with high energy and power densities.

This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

F13: Hybrid Graphene/Carbon Nanotube Films as Transparent Conductors

Çolak, Fatma (Istanbul Technical University, Istanbul, TUR); Tabatabaei Mohseni, Amin (Istanbul Technical University, Istanbul, TUR); Karatepe, Nilgün (Istanbul Technical University, Istanbul, TUR)

The need for transparent conductive films (TCFs) is growing rapidly as optoelectronic devices, such as touch screens, displays, and photovoltaics become essential in our lives. Due to their remarkable electrical, optical and mechanical properties carbon

nanomaterials (carbon nanotubes (CNTs) and graphene) are extensively researched as transparent electrodes for optoelectronic applications. Hybridized CNT-Graphene networks can exhibit superior optoelectronic properties than individual nanomaterials. In this work, Tuball Single-Walled CNTs were purchased from OCSiAl company and graphene was synthesized by Modified Hummers method. Hybrid CNT-Graphene networks were fabricated on flexible substrates by simple ultrasonic spray coating deposition technique. The effects of different configurations (Graphene/CNT, CNT/Graphene, Graphene/CNT/Graphene) on film morphology and optoelectronic properties of films were investigated.

F14: Improvement of Surface Properties of VACNT/MoO_x Buffer Layer for High Efficient Solar Cells

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One of the unusual structure of the element carbon, the carbon nanotubes (CNT) which formed since 1991 with outstanding features has been at the center of the scientific world. Carbon nanotubes have excellent electrical, mechanical, thermal and chemical properties and due to their multifaceted nature they are materials which have applications in different fields. Depending on the properties desired in commercial applications, carbon nanotubes can be produced in bulk or thin film form. Vertically aligned carbon nanotubes (VACNT) which are carbon nanotubes grown on a substrate creates a CNT thin film and modifications can be made on this surface. Studies conducted in recent years shows us that micro-nano biomimetic hierarchical structures which are often used inorganic thin films can also be made with carbon nanotubes. Thus, with the unique features of carbon nanotubes advantages of hierarchical structure to systems is further improved. Vertically aligned periodic arrays of carbon nanotubes are used to create the micro-, submicro-, and nanoscale roughness on different layers of solar cells to ensure good contact with metal oxide layers such as MoO_x buffer layer. Improved surface properties and good electrical characteristics are suitable for ensuring enough efficiency improvement in carbon based solar cells. In this work, chemical vapour deposition method applied for production of vertically aligned multiwalled carbon nanotubes with using layer by layer catalysts system. Then the surface properties of MoO_x combined carbon nanotube buffer layer were characterized for efficiency improvement in solar cell structure. Characterization of VACNT/MoO_x buffer layer is performed using Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Raman Spectroscopy and electrical measurements.

F15: Lithium-ion storage with nanotube-bound porous silicon

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Lithium-ion battery technology has found many applications in everyday devices, but there remain significant challenges in increasing the energy density and (dis)charge rate of these cells. The graphite anodes used in commercially available Li-ion batteries are not optimal for storing the lithium ions in the charged cell, since elemental silicon has a tenfold theoretical capacity [1]. Unfortunately, silicon expands in volume when alloyed with lithium, which destroys its mechanical structure with continued cycling, causing lower conductivity and capacity. This problem can be partly circumvented by using either nanosized or porous silicon particles, but the conductivity of an anode made only of such materials is low, making the use of binders [2] or conductive additives necessary. Our study aims to enlarge the capacity of the anode by using mesoporous silicon particles [3], and improve its conductivity and mechanical stability by linking the particles with a carbon nanotube-polymeric binder composite. Covalent linking of the CNTs and the silicon particles becomes possible through amide bonding [4]. Layer-by-layer assembly with polyelectrolytes helps in both dispersing single-walled CNTs and subsequently in conjugating them together, producing a stable and conducting binder structure. Different amounts of both SWCNTs and MWCNTs, particle sizes as well as two conjugation approaches are tested to optimize the material. Helium ion microscopy is used to produce swelling in silicon particles with simultaneous characterization, simulating the stresses of cell operation in the anode material.

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F16: Micro-supercapacitor with High Areal Energy Density of Blade-coated Porous Single-walled Carbon Nanotube Electrodes

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Micro-supercapacitors have been developed into miniaturized and planar devices as a new emerging branch of supercapacitors due to the growing interest in portable and wearable electronic devices. Besides the benefit for feature size, miniaturization contributes to high frequency response and charge/discharge speed by enhancing the ion-accessibility to the surface of the electrodes and allows designable performance by integration into series-parallel circuits. However, the relatively low areal charge stored in micro-supercapacitors precludes the applications requiring high energy densities. Here we propose the fabrication technique of micro-supercapacitors enabling high areal capacitance for carbon nanotube electrodes by combining blade coating and patterning by lithography. We have developed the blade coating

technique of single walled carbon nanotube films covering wide range of film thickness and controlling the pore structure and specific surface area. The process is compatible with conventional lithography techniques and suited for the full device integration. We will present the performance of the supercapacitor of the CNT electrodes with different porous structure and film thickness. We will propose the way of obtaining high areal energy density with discussing the influence of porous structure on the ion transport resistance. This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

F17: Performance Enhancement of Polymer-Free Carbon Nanotube Solar Cells via Transfer Matrix Modeling

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Polymer-free (6,5) single-walled carbon nanotubes (SWCNTs) prepared using the gel permeation approach are integrated into SWCNT:C 60 solar cells. Evaporation-driven self-assembly is used to form large-area SWCNT thin films from the surfactant-stabilized aqueous suspensions. The thicknesses of various layers within the solar cell are optimized by theoretical modeling using transfer matrix calculations, where the distribution of the electric field within the stack is matched to light absorption by the SWCNTs through either their primary (S 11) or secondary (S 22) absorption peaks, or a combination thereof. The validity of the model is verified experimentally through a detailed parameter study and then used to develop SWCNT:C 60 solar cells with high open-circuit voltage (0.44 V) as well as a cutting-edge internal quantum efficiency of up to 86% through the nanotube S 11 transition, over an active area of 0.105 cm².

F18: Polymer functionalized carbon nanotubes as highly active catalysts for electrochemical hydrogen production

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Among different methods to produce hydrogen as the future clean energy carrier, electrochemical water splitting is a promising straightforward method. However, current electrochemical electrolyzers utilize expensive and scarce noble metal electrocatalysts retarding adoption of this technology. Therefore, development of efficient and low-cost electrocatalyst for hydrogen and oxygen evolution reactions (HER and OER) occurring on the cathode and anode of an electrochemical

electrolyzer, respectively, are required. Consequently, efficient non-noble metal [1, 2] and metal free [3, 4] electrocatalysts have been introduced for these reactions recently. The unique structure and intrinsic properties of carbon nanotubes (CNTs) such as high-surface area, high-chemical stability, and high electrical conductivity make them extremely attractive as catalyst supports for heterogeneous electrochemical catalysis. Thus, synthesis of composite materials of CNTs has been selected in this study as a promising approach to fabricate efficient and low-cost electrocatalysts. Functionalization of CNTs with low-cost polymers is a novel and relatively simple method to fabricate metal free catalysts for HER and OER in electrochemical water electrolysis. The fabricated composite materials, based on the combination of CNTs and polymers, have shown properties of the individual components with synergistic effects [5]. These metal free electrocatalysts show catalytic properties toward both HER in acidic media and OER in alkaline environment comparable to those of commercial noble metal based electrocatalysts. This work opens new avenues for the functionalization of CNT with polymers in order to synthesize new catalyst materials for the electrochemical hydrogen production.

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F19: Probing the Limit of Single Walled Carbon Nanotubes in Polymer-Free SWCNT-Fullerene C₆₀ Solar Cells

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In this work, single walled carbon nanotube SWCNT:C₆₀ solar cells from monochiral small and large diameter nanotubes along with polychiral mixtures were prepared. Through assignment of the different nanotube chiralities from photoluminescence (PL) and optical density measurements a diameter limit yielding 0 % IQE was determined. This work provides insights into the required net driving energy for SWCNT exciton dissociation onto C₆₀ and establishes a family of (n,m) species which can efficiently be utilised in polymer free SWCNT:C₆₀ solar cells. Using this approach the largest diameter nanotube with an IQE > 0 % was found to be (8,6) with a diameter of 0.95 nm. Possible strategies to extend this diameter limit are then discussed.

F20: Production of N-functionalized carbon nanodots by carbonization of leaves, and evaluation of their photoluminescence properties

Sandström, Robin (Umeå University - Department of Physics, UMEÅ, SWE)

Nano-sized carbon materials with defined morphologies have wide spectra of applications. Carbon nanodots (Cdots) are however seen as a class of material where an extended range of uses are predicted. In particular, fluorescent Cdots have shown potential in not only bioimaging and biosensing, but also for various catalytic purposes as it is a highly multifunctional compound. Here we produce high yields of fluorescent Cdots with a surprisingly overlooked natural eco-friendly carbon source; plant leaves. The synthesis procedures include a simple hydrothermal treatment for efficient carbonization of the biomass, resulting in non-graphitic crystalline Cdots with an average size of roughly 5nm as well as an additional product of around 20nm as evidenced by High resolution transmission electron microscopy (HRTEM). Attempts of understanding the particle formation by analyzing the waste products as well as characterization of optical properties of the resulting dispersions are emphasized. Fourier transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) suggests that our products are heavily functionalized with various N - and hydrophilic oxygen groups. Further, their highly fluorescent behaviors under UV illumination are noted.

F21: Three-Dimensional Graphene Network - Polypyrrole Nanowire Arrays Hybrid Material for Supercapacitor Electrode

Ma, Yuxiao (Beihang University, Beijing, CHN); Yu, Mei (Beihang University, Beijing, CHN); Liu, Jianhua (Beihang University, Beijing, CHN)

High-conductive carbonaceous materials and pseudocapacitance materials are used comprehensively in supercapacitor to get high rate capability and good cycling performance. Herein, we report a three-dimensional(3D) graphene network - polypyrrole (PPy) nanowire arrays hybrid material. Vertically aligned polypyrrole nanowire arrays are synthesized on 3D graphene network by a template-free electrodeposition method, and its potential application as supercapacitor electrode is explored. The fabrication of 3D graphene network-PPy nanowire arrays requires two steps. In the first step, 3D graphene network was prepared by chemical vapor deposition(CVD) of graphene on nickel foam, which was followed by the etching of nickel framework. In the second step, vertically aligned PPy nanowire arrays were electrodeposited on 3D graphene network by potentiostatic method with a potential of 0.721V (vs. Ag/AgCl). The forming of PPy nanowire arrays morphology is attributed to the electrostatic repulsion between grown individual PPy nanowires. 3D graphene network is an intact, interconnected, and highly conductive network instead of separated sheets. It serves as current collector in the material. Its good conductivity prevents the charges generated by pseudocapacitive reaction from accumulating on PPy nanowires, and thus, the structure demolishment and performance degradation caused by electrostatic force can be minimized. The vertically aligned nanowire morphology increases the specific area of PPy, and thus

contributes to the charge transfer between electrolyte and electrode. The space between nanowires provides unblocked diffusion path for electrolyte ions, and facilitates the protonation and deprotonation process of PPy. These factors promote the capacitance performance of the material, including high specific capacitance, good high-rate performance, and high cyclic stability.

F22: Vertically aligned carbon nanotubes based materials for high energy hybrid supercapacitors

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The aim of this project is to develop innovative electrodes materials with high specific capacitance based on vertically aligned carbon nanotubes (VACNT) to be included in supercapacitors with improved specific energy. To achieve this, we will develop new pseudocapacity positive electrode materials based on vertically aligned carbon nanotubes (VACNT) modified by Electronic Conducting Polymers (ECP) and/or manganese oxide electrodeposited in a controlled manner. In this study, the growth of VACNT by catalytic chemical vapour deposition using mixed aerosol [1] has been adapted for different metal substrates (stainless steel or Al) with controlled and optimized morphologies (length, density, diameter...). VACNT are then used as electrode support material through the development of preparation methodologies of various VACNT/PCE nanocomposite electrodes through electrochemical polymerization with various techniques on VACNT carpets used as templating electrode [2]. VACNT are also used as the 3D matrix hosting the electrodeposition of nanostructured MnO₂ with the objective to optimize the electrochemical parameters in order to deposit the oxide homogeneously throughout the entire depth of the carpet. The electrodeposition is performed in different media and from different MnO₂ precursors [3]. Several pre-treatments of the VACNT with oxygen have been thus performed to act on the hydrophobic character of the pristine forest. Oxide film growth by CVD has also been tested. The materials and composites have been characterized by scanning and transmission electron microscopies as well as spectroscopies (SEM, TEM, Raman, SEM-EDX and XPS) in order to examine the morphology, the localization and the thickness of the PCE or MnO₂ deposits and their relation to the measured specific capacitance performances.

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F23: Vertically-Aligned Silicon Carbide Nanowires as Metal-Free Photocatalyst

Hong, Jindui (University of Oxford, Oxford, GBR); Meysami, Seyyed Shayan (University of Oxford, Oxford, GBR); Holdway, Philip (University of Oxford, Oxford, GBR); Grobert, Nicole (University of Oxford, Oxford, GBR)

Nanomaterials with designed structure are vital to meet requirements necessary for their efficient exploitation in photocatalytic applications. Next generation photocatalysis is considered to be one of the feasible strategies related to the emerging energy and environmental challenges. Silicon carbide (SiC) is one of most promising photocatalysts due to its variable band gap, high electron mobility and high conduction band. SiC nanowires with aligned structure have further benefits including better electron and mass transfer which control the photocatalytic efficiency. Here, we report the large scale synthesis of new vertically-aligned silicon carbide nanowires (VASiC) by using vertically-aligned carbon nanotube (VACNT) templates which also act as a C source. In order to generate VASiC, VACNT matrix material was infiltrated with a silica precursor using a sol-gel method and then reacted with VACNT and Si powder. The crystallinity, structure, thermal stability, and light absorbance of VASiC were systematically characterised. It was found that the as-synthesised VASiC are ca. 1 mm thick (e.g. length of individual SiC fibres), have diameters of 50-90 nm, and exhibit a cubic crystal structure. Their light absorbance is strong (up to 600 nm) while their band gap was estimated to be 2.15 eV. The results of photocatalytic Rhodamine B (RhB) degradation showed that the VASiC can decompose the RhB efficiently (90% removal within 30 min) without adding any noble metal cocatalyst, demonstrating its promising application as metal-free photocatalyst.

Program for Wednesday, August 10th 2016

09:00 - 9:30	Invited Talk: Andrea Goldoni <i>Nanostructured Carbon-based Materials for Gas Sensor Applications</i>
09:30 - 09:45	Contributed Talk: Giacomo Argentero <i>Analysis of graphene-hBN heterostructures by high-resolution scanning transmission electron microscopy with direction-sensitive detection of scattered electrons</i>
09:45 - 10:00	Contributed Talk: Etienne Gaufrès <i>Isothermal Encapsulation of α-sexithiophene in Single-Walled Carbon Nanotubes</i>
10:00 - 10:30	Invited Talk: Ramakrishna Podila <i>Defect-engineered nanocarbons for electrochemical energy storage</i>
10:30 - 10:45	Contributed Talk: Alexey Cherevan <i>Nature and extent of charge/energy transfer at the nanocarbon-metal oxide interface</i>
10:45 - 11:15	Coffee Break
11:15 - 11:45	Invited Talk: L. Chang <i>Selective growth of semiconducting and metallic single-wall carbon nanotubes</i>
11:45 - 12:00	Contributed Talk Laurent Alvarez <i>Modulating single-walled carbon nanotube opto-electronic properties by chromophore confinement</i>
12:00 - 12:30	Invited Talk: Hirofumi Kataura <i>Large scale separation of single-chirality single-wall carbon nanotubes using gel column chromatography</i>
12:30 - 12:45	Contributed Talk: Katalin Kamarás <i>Cloaking of encapsulated molecules in carbon nanotubes at infrared frequencies</i>
12:45 - 13:15	Conference Photo
13:15 - 14:00	Pack Lunch @ Arkadenhof
14:15	Conference Tour
18:00	Banquet

WEDNESDAY

135

IT4: Nanostructured Carbon-based Materials For Gas Sensor Applications

Goldoni, Andrea (Elettra, Trieste, ITA)

Here we present the nano-structured carbon based materials for sensors applications. Characteristics that suggest nano-structures as promising candidate for extremely sensitive gas sensors are the high-active surfaces and high- aspect ratios as well as the low cost of production and the large changes in the electronics properties due to a very tiny external perturbations. Moreover, possible integration in everyday life devices with scalability and portability will be another application to take into consideration. Carbon Nanotubes, carbon/metals and carbon/metal-oxides nano-systems are quite interesting to produce chemiresistor gas sensors with high sensible (sub-ppm), stable and a fast recovery time for environmental monitoring

CT12: Analysis of graphene-hBN heterostructures by high-resolution scanning transmission electron microscopy with direction-sensitive detection of scattered electrons

Argentero, Giacomo (Physik Nanostrukturierter Materialien, Wien, AUT); Mittelberger, Andreas (Physik Nanostrukturierter Materialien, Wien, AUT); Cao, Yang (Department of Physics and Astronomy, University of Manchester, Manchester, GBR); Kotakoski, Jani (Physik Nanostrukturierter Materialien, Wien, AUT); Mangler, Clemens (Physik Nanostrukturierter Materialien, Wien, AUT); Pennycook, Timothy (Physik Nanostrukturierter Materialien, Wien, AUT); Kramberger, Christian (Physik Nanostrukturierter Materialien, Wien, AUT); Geim, Andre K. (Department of Physics and Astronomy, University of Manchester, Manchester, GBR); Meyer, Jannik C. (Physik Nanostrukturierter Materialien, Wien, AUT)

In recent years, heterostructures of 2-D materials have gathered significant attention [1]. Since graphene and hBN have nearly the same lattice constant, structural distortions can appear if the orientation of the lattices is aligned [2]. Here, we investigate a free-standing, orientationally aligned graphene and single-layer hBN heterostructure by electron microscopic methods. In particular, we used electron diffraction and dark-field TEM imaging to evaluate the global structure as well as aberration-corrected scanning transmission electron microscopy (STEM) to study the local atomic arrangements. Besides standard annular dark field (ADF) imaging, we developed a detection scheme where a pixelated detector is used to record not only the total scattered intensity but also the direction of the scattered intensity in its angle and magnitude. This signal is very sensitive to the relative position of atoms on top of each other in the two layers of the sample, as verified also by simulated data. Fig. 1 shows a medium-angle ADF image of a heterostructure with only 1° orientational misalignment. Different local stacking configurations can be identified within the moiré. AB stacked regions consistently appear larger than AA or AB' stacked areas, which is clear evidence for a structural distortion due to the interaction between the layers. Current work in progress is to reconcile these observations with theoretical models, in order to understand the in-plane (shear, strain) and out-of-plane (bending) components of the observed distortion as well as to gain insight to the underlying interaction between the sheets.

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CT13: Isothermal Encapsulation of α -sexithiophene in Single-Walled Carbon Nanotubes

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Here, we capitalize on the giant Raman scattering effect from 1D aggregated dye molecules [1] to probe the encapsulation process of molecules into carbon nanotubes. The isothermal encapsulation is followed at 30°C and 115°C by Raman spectroscopy and hyperspectral Raman imaging. The analysis of the isotherms shape coupled to the encapsulation profile imaging of long SWCNT allow us to highlight the filling and assembling scenario of α -sexithiophene (6T) into SWCNT with diameters of 1.35 ± 0.2 nm. [2] The Raman experimental data are fitted using both a Langmuir (type VI) and Ising isotherm models. We show that 6Ts encapsulate from the nanotube ends and assemble spontaneously as single-aggregates, then as pair-aggregates with a formation enthalpy $\Delta H_{\text{pair}} = -260 \pm 20$ meV per molecule.

[1] Giant Raman scattering from J-aggregated dyes inside carbon nanotubes for multispectral imaging.

E. Gaufrès, N Y-W Tang, R. Martel et al. Nature Photonics (2014)

[2] Isothermal Encapsulation of α -sexithiophene in Single-Walled Carbon Nanotubes

E. Gaufrès, N Y-W Tang, R. Martel et al. (submitted)

IT5: Defect-engineered nanocarbons for electrochemical energy storage

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Today's batteries and electrochemical capacitors, which are the main components for energy storage, do not have sufficiently high energy and power densities to store and appropriately discharge the energy from traditional renewable energy sources or to power long-range electric vehicles. Nanocarbons (NCs) such as carbon nanotubes and graphene are excellent electrode materials for electrochemical capacitors due to their economic viability, high-surface area, and high stability. However, the net amount of energy stored in NC-based capacitors is much below the theoretical limits due to two inherent bottlenecks: i) their low quantum capacitance, and ii) limited ion-accessible surface area. Contrary to the notion that defects are performance limiters, we found defects in NCs to be critical for overcoming the intrinsic bottlenecks and opening new channels for ion diffusion. This talk will summarize recent advances from Clemson Nanomaterials Center in defect-engineered NC supercapacitors, which are now able to reach energy densities of 500% higher than the state-of-the-art supercapacitors

CT14: Nature and extent of charge/energy transfer at the nanocarbon-metal oxide interface

Cherevan, Alexey (Technische Universität Wien, Vienna, AUT); Kemnade, Nina (Westfälische Wilhelms-Universität Münster, Münster, GER); Gebhardt, Paul (Technische Universität Wien, Vienna, AUT); Wilde, Gerhard (Westfälische Wilhelms-Universität Münster, Münster, GER); Eder, Dominik (Technische Universität Wien, Vienna, AUT)

Nanocarbon-inorganic hybrids constitute a novel class of composite materials that have recently attracted considerable attention for use in applications where efficient charge extraction is required. Key to these hybrids is the rational hybridization of two complementary compounds, i.e. a nanocarbon and an active inorganic nanomaterial, in a way that creates tight interface between them. Such hybridization enhances interfacial charge and energy transfer processes, which in turn can further facilitate efficient charge separation and extraction. So far the majority of published works in this field have merely assumed the presence of charge transfer in nanocarbon containing hybrids and only few have tried to experimentally evaluate these processes e.g. by using fluorescence quenching. These works, however, have not considered potential energy transfer process as well as light absorption and scattering by the nanocarbon. Furthermore, the reported samples showed non-attached metal oxide agglomerates and non-uniform morphology, which does not allow for accounting for other quenching contributions such as inter-particle quenching and particle size effects. In this work we have designed a unique model system that allowed for reliable and in-depth investigations of interfacial charge and energy transfer in nanocarbon hybrids. We used a modified atomic layer deposition (ALD) process to create new sandwich structures comprising of a central carbon nanotube (CNT) core, thin films of Al_2O_3 and a decorating layer of photoluminescent ZnO nanoparticles. The novelty of our model originates from the introduction of a dielectric barrier layer between the hybrid components with atomically precise control of thickness varied between 2 nm and 100 nm. This has, for the first time, allowed for distance-dependent photoluminescence quenching studies in CNT containing nanocarbon hybrids and provided some intriguing mechanistic findings.

IT6: Selective growth of semiconducting and metallic single-wall carbon nanotubes

Liu, Chang, (Shenyang National Laboratory of Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China)

Single-wall carbon nanotubes (SWCNTs) can be either semiconducting or metallic, depending on their diameters and chiral angles. Semiconducting SWCNTs (s-SWCNTs) are potential channel material of high-performance field effect transistors with advantages of high carrier mobility and excellent flexibility; metallic SWCNTs can be used as interconnectors in circuits. Usually, as-prepared SWCNTs are a mixture of s- and m-SWCNTs. Therefore, it is highly important to prepare pure SWCNTs with uniform electrical types to achieve their use in electronics. In this presentation, we report the direct growth of high-quality s- and m-SWCNTs by a floating catalyst chemical vapor deposition (FCCVD) method and by novel catalyst design. We introduce suitable amount of oxygen or hydrogen as etchant during the growth of SWCNTs by the FCCVD method. As a result, SWCNTs with higher chemical reactivity are selectively removed, and enriched s- and m-SWCNTs are obtained in large scale. On the other hand, we design and prepared novel catalyst with superior stability compared to traditional transition metals, and obtained SWCNTs with a narrow band gap distribution.

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CT15: Modulating single-walled carbon nanotube opto-electronic properties by chromophore confinement

Lahjiri, Fayçal (Laboratoire Charles Coulomb, Montpellier, FRA); Cassabois, Guillaume (Laboratoire Charles Coulomb, Montpellier, FRA); Izard, Nicolas (Laboratoire Charles Coulomb, Montpellier, FRA); Joussetme, Bruno (Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences, Gif-sur-Yvette, FRA); Campidelli, Stéphane (Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences, Gif-sur-Yvette, FRA); Saito, Takeshi (National Institute of Advanced Industrial Science and Technology, Tsukuba, FRA); Lauret, Jean-Sébastien (Laboratoire Aimé Cotton, Orsay, FRA); Delpont, Géraud (Laboratoire Aimé Cotton, Orsay, FRA); Bantignies, Jean-Louis (Laboratoire Charles Coulomb, Montpellier, FRA); Alvarez, Laurent (Laboratoire Charles Coulomb, Montpellier, FRA)

Opto-electronic properties of single-walled carbon nanotubes can be significantly modified by chromophore confinement into their hollow core. For instance, charge transfers are evidenced from Raman data analysis. First, by exciting nanotubes far from the optical absorption of the molecule, the Raman G-band signal exhibits a weak but significant up or downshift depending on the nanotube diameters. This behavior is consistent with a permanent electron transfer to the nanotube in the framework of the renormalization process [1]. In addition, close to the molecule resonance, the magnitude of the G-band shift is enhanced for small diameter tubes, evidencing a photo-induced electron transfer. Finally, the Breit-Wigner-Fano lineshape (characteristic of electron-phonon coupling) of the Raman G-band can be strongly reduced for defective metallic nanotubes. After molecule functionalization, this peculiar profile is recovered, suggesting a back donation of electrons to the nanotube. Photoluminescence properties of semiconducting nanotubes are also significantly modified by chromophore confinement. The nanotube emission intensity is amplified after encapsulation. This exaltation depends on the nanotube diameter, and can be related to diameters exactly fitting the molecule size. The origin of the photoluminescence enhancement will be discussed.

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IT7: Large scale separation of single-chirality single-wall carbon nanotubes using gel column chromatography

Kataura, Hiromichi (NMRI, AIST, Tsukuba, JPN)

Because single-wall carbon nanotubes (SWCNTs) have structural flexibility, structure controlled synthesis is still very difficult. On the other hand, since physical properties of SWCNT is highly dependent on its structure, structure sorted SWCNT is highly desired especially for the electronic and opt-electronic device applications. Many structure sorting methods have been developed to date, but most of them are still within a laboratory scale. For the industrial use, we need really scalable sorting technology. In this work, we demonstrated to separate (9,4) and (10,3) single-chirality SWCNTs using one-step adsorption chromatography with mg/day scale [1]. Where, we used two different structure selections in the adsorption and desorption process, respectively. Furthermore, we can extend our method to the other chiralities. Since all materials and equipment used in this work were on the market, anybody can repeat our method easily. This repeatability is very important for industrial applications.

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CT16: Cloaking of encapsulated molecules in carbon nanotubes at infrared frequencies

Kamarás, Katalin (Wigner Research Centre for Physics, Budapest, HUN); Pekker, Áron (Wigner Research Centre for Physics, Budapest, HUN); Tóháti, Hajnalka (Wigner Research Centre for Physics, Budapest, HUN); Botka, Bea (Wigner Research Centre for Physics, Budapest, HUN); Walker, Kate (University of Nottingham, Nottingham, GBR); Khlobystov, Andrei (University of Nottingham, Nottingham, AUT); Hackl, Rudi (Walther-Meissner-Institute, Garching, GER); Nishimura, Yoshifumi (Waseda University, Tokyo, JPN); Witek, Henryk (National Chiao Tung University, Hsinchu, TWN); Irlé, Stephan (Nagoya University, Nagoya, JPN)

The construction of an electromagnetic “invisibility cloak” usually involves a medium with spatially varying optical properties, i.e. a metamaterial. The topic of this contribution is a cloaking mechanism based on electromagnetic shielding by polarizable electrons in real materials. Molecules encapsulated in carbon nanotubes become invisible to infrared radiation because of the mirror charges invoked in the nanotube wall during molecular vibrations. I will present experimental data and results of model calculations on this phenomenon.

Program for Thursday, August 11th 2016

09:00 - 9:45	Key Note Lecture: Tony Heinz <i>Two-dimensional semiconductors: The counterpart to graphene</i>
09:45 - 10:00	Contributed Talk: Van Luan Nguyen <i>Wafer scale single-crystalline AB-stacked bilayer graphene</i>
10:00 - 10:30	Intro Posters G&H: Riichiro Saito
10:30 - 12:00	Coffee Break & Poster Session
12:00 - 12:30	Invited Talk: Yutaka Ohno <i>Carbon nanotube flexible/stretchable devices for wearable electronics</i>
12:30 - 12:45	Contributed Talk: Georgy Fedorov <i>Carbon nanotube based devices for terahertz applications.</i>
12:45 - 13:00	Contributed Talk: Gabriela Borin Barin <i>Bottom-up fabrication of graphene nanoribbons: From molecules to devices</i>
13:00 - 14:15	Lunch
14:15 - 14:45	Invited Talk: Y. Chen <i>Tailoring Carbon Nanomaterials for Emerging Applications</i>
14:45 - 15:00	Contributed Talk: S. Satoro <i>THz spectroscopy of graphene complementary split ring resonators</i>
15:00-15:15	Contributed Talk: Kazuhiro Yanagi <i>Tuning Thermoelectric Properties of Single Wall Carbon Nanotubes by Electric Double Layer Carrier Injection</i>
15:15 - 15:30	Contributed Talk: Win Wenseleers <i>Asymmetric dye-filled carbon nanotubes for nonlinear optics</i>
15:30 - 16:00	Intro Posters I/J: Milo Shaffer
16:00 - 17:30	Refreshments /Posters
17:30	Walking Tour

THURSDAY

KN4: Two-dimensional semiconductors: The counterpart to graphene

Heinz, Tony; Depts. of Applied Physics and Photon Science, Stanford University, Stanford, CA 94305, USA and SLAC National Accelerator Laboratory, Menlo Park, CA USA 94025, USA

We will review recent progress in understanding the electronic and optical properties of a new class of 2D semiconductors, monolayers of transition metal dichalcogenides in the MX_2 class ($M=Mo, W$; $X=S, Se$). These materials provide an excellent complement to the metallic 2D system of graphene, in which, unlike in the case of carbon nanotubes, it is challenging to create a large band gap.

These 2D semiconductors, which are stable under ambient conditions, can be readily employed as field-effect transistors with large on-off ratios. They have, moreover, been shown, in contrast to their bulk counterparts, to exhibit direct-gap character as monolayers. They are thus efficient nanoscale light emitters. In addition, the materials exhibit remarkably strong and distinctive excitonic interactions, associated with the reduced dielectric screening in the two-dimensional limit. This is manifest in the stability not only of excitons, but also of three (trion) and four (biexciton) states. The materials have also been shown provide a route to access the valley degree of freedom through selection rules for valley-selective excitation using circularly polarized light. Further, the existence of an ever-widening class 2D van der Waals materials offers exciting possibilities for the creation of novel heterostructures of layers with tunable electronic properties different from either of the constituents.

CT17: Wafer scale single-crystalline AB-stacked bilayer graphene

Nguyen, Van Luan (SKKU, Suwon, KOR); Lee, Young Hee (SKKU, Suwon, KOR)

While a lot of efforts on preparing large area AB-BLG using Cu or Cu-Ni alloy substrate via chemical vapor deposition method have been reported, the obtained BLG is polycrystalline with the grain size still limit in micrometer-scale and bilayer region is partially achieved because the catalytic activity of the Cu surface is suppressed by the presence of monolayer. Because of these critical difficulties, we introduce a new concept to form wafer-scale single-crystalline AB-BLG. Firstly, wafer-scale single-crystalline monolayer graphene (MLG) was prepared on single crystal Cu(111) film via seamless stitching concept that we have reported (Adv. Mater. **27**, 1376-1382, (2015)). The Cu(111) film was grown on 2" sapphire via conventional RF-magnetron sputtering which requires a narrow growth temperature zone and the use of single crystal Cu(111) target. The obtained Cu(111) film is ultra-flat (RMS of 1.8 Å) and stacking-faultless, a key issue to synthesize single-crystalline MLG. This MLG is then aligned transfer onto another MLG, while second MLG remains on the initial Cu(111) film. This process allows exact alignment and polymer-free interface between two layers, resulting in wafer-scale single-crystalline AB-BLG that is electronically equivalent to exfoliated BLG. Evidence of AB-BLG is supported via transmission electron microscopy, angle-resolved photoemission spectroscopy, quantum Hall Effect and self-consistent effective mass characterization. Clear plateaus and quantum steps following fourfold degenerate steps with well-defined Landau filling factors. From 2D mapping of Hall resistance vs. magnetic field and gate voltage, we observed a clear Landau fan for AB-BLG, consistent with those from exfoliated samples. The wafer-scale single-crystalline of artificial AB-BLG is confirmed by low energy electron diffraction pattern and further demonstrated by integrating 380 dual-gate FET devices on a 2 x 2 cm² wafer. 96.5% devices show AB-stacking behaviour and median carrier mobility of 2200(±200) cm²/Vs.

IT8: Carbon nanotube flexible/stretchable devices for wearable electronics

Yutaka Ohno, Institute of Materials and Systems for sustainability, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan.

Flexible, body-worn healthcare/medical devices have the potential to revolutionize preventive medical care and health promotion. Carbon nanotube thin films are promising electronic materials for transistors [1-3], biosensors [4,5], and other passive components to build such flexible devices because of the excellent electronic and mechanical properties and biocompatibility. In the presentation, our recent works on flexible transistors and biosensors based on carbon nanotube thin films will be introduced, including high-mobility thin-film transistors and integrated circuits on a flexible plastic film, extremely stretchable thin-film transistors, wafer-scale assessment of uniformity in their property, electrochemical biosensors with high-sensitivity and stability, thin-film transistor-based potentiometric biosensors with ultra-high sensitivity and wide dynamic range, and so on.

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CT18: Carbon nanotube based devices for terahertz applications

Fedorov, Georgy (Moscow Institute for physics and Technology, Dolgoprudny, RUS); Gayduchenko, Igor (Moscow State Pedagogical University, Moscow, RUS); Goltsman, Gregory (Moscow State Pedagogical University, Moscow, RUS)

Increased sensitivity of detection of terahertz (THz) signals can be achieved by reducing the size of the sensitive element. Therefore, it is expected that recent advances in nanotechnology may result in cost-effective solutions for new THz detectors. One particular route is the use of carbon nanotubes (CNTs) that can be easily synthesized in a chemical vapor deposition (CVD) system using inexpensive precursors for the growth. This talk will be devoted to the prospects of using asymmetric CNT devices as a basic element of THz detectors. We studied response of such devices to terahertz radiation [1, 2]. It was maintained that photothermoelectric effect under certain conditions results in strong response of such devices to terahertz radiation even at room temperature. The asymmetry which is crucial for the observation of the DC voltage response to the radiation has been implemented in our devices in different ways. In most cases different metals are used to contact the CNT network of a uniform morphology at the source and drain electrodes. Such devices show the most promising results with room temperature responsivity of up to 100V/W. Analysis of the experimental data shows that the response contains two components. One is thermal reflecting different increase in temperature in the areas of the nanotube/metal interfaces. The second is a response due to the non-linearity of the current-voltage characteristic of the device at zero bias. The rectification of the signal leads to a DC component, which contributes to the observed signals. This work was supported by the Grant of Ministry of Education and Science of Russian Federation under Contract No. 14.586.21.0003 (project ID RFMEFI58614X0003).

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CT9: Bottom-up fabrication of graphene nanoribbons: From molecules to devices

Borin Barin, Gabriela (EMPA, Dübendorf, CHE); Fairbrother, Andrew (EMPA, Dübendorf, CHE); Sanchez-Valencia, Juan Ramon (EMPA, Dübendorf, CHE); Llinás, Juan Pablo (UC Berkeley, California, USA); Feng, Xinliang (TU Dresden, Dresden, GER); Mullen, Klaus (Max Planck Institute for Polymer Research, Mainz, GER); Ruffieux, Pascal (EMPA, Dübendorf, CHE); Paillet, Matthieu (Université de Montpellier, Montpellier, FRA); Bokor, Jeffrey (UC Berkeley, California, USA); Fasel, Roman (EMPA, Dübendorf, CHE)

Atomically precise graphene nanoribbons (GNRs) exhibit a sizeable bandgap, and thus potentially overcome many of the limitations of graphene in electronic device applications. However, in spite of their exceptional properties, significant challenges remain for GNR fabrication, processing and characterization¹. Bottom-up synthesis of graphene nanoribbons² is most commonly performed under ultra-high vacuum conditions, which are difficult to maintain in an industrial setting. Additionally, little is known about the stability of ultra-narrow GNRs under ambient conditions or during device processing. This contribution addresses some of these challenges, in particular regarding GNR fabrication scalability, characterization, and device fabrication. On-surface synthesis from molecular precursors was focused on 7- and 9-AGNRs (7 and 9 carbon atoms wide GNRs with armchair edges, respectively) on 200nm Au(111)/mica substrates, under high to ultrahigh vacuum conditions. 7-AGNRs were found to be stable for several months under ambient conditions, with minor alterations to the Raman characteristics of the ribbons. The most notable changes were an increase in the full-width-at-half-max of all peaks and a blue-shift of the G-peak, which we ascribe to intercalation of water between the GNRs and the metal substrate. Detailed studies including polarized and multi-wavelength Raman characterization of 7- and 9-AGNRs will be discussed. Concerning device application, field effect transistors (FET) fabricated with 7-AGNRs have shown low drive current of 1 nA for 1 V drain bias due to large Schottky barriers at the contacts caused by the large band gap of 7-AGNRs ($>3\text{eV}$)³. Due to their significantly lower band gap ($\sim 2.1\text{eV}$), 9-AGNRs demonstrate a two orders of magnitude improvement with 100 nA of on-current and on-off ratios $>10^3$ which can potentially improve the on-state performance of GNR-FETs⁴.

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IT9: Tailoring Carbon Nanomaterials for Emerging Applications

Chen, Yuan; School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, Australia

Carbon nanomaterials have many extraordinary properties, which depend on their unique nanoscale structures. There are two major challenges in realizing their potential applications. First, it is difficult to produce carbon nanomaterials with precisely controlled nanoscale structures in large quantity. Second, carbon nanomaterials often lose their desired properties observed in nanoscale when used as the building block of macroscopic systems. This talk covers our research efforts on addressing these two challenges in three areas.

First, several sulfur doped cobalt catalysts were developed to grow semiconducting (9,8) single walled carbon nanotubes with good production scalability. We found sulfur affects the nucleation and catalytic activity of metal catalyst particles. The impacts of sulfur in single walled carbon nanotube synthesis can be controlled to modulate chirality selectivity and carbon yield.¹⁻⁴ Second, we used capillary columns and space-confined channels as hydrothermal reactors to assemble graphene oxide sheets and carbon nanotubes into unique multiscale hierarchical structured hybrid fibers, which shows high volumetric capacitance. The hybrid carbon fibers were used to construct fiber supercapacitors. These devices can cover a wide range of energy and power needs, and they demonstrate good potentials as energy storage solutions for wearable and implantable devices.⁵⁻⁸ Third, graphene oxide sheets were used to modulate properties of polymeric hollow fiber membranes for water treatment. Further, versatile carbon architectures were designed by intercalating surface-functionalized, small-diameter, multi-walled carbon nanotubes into reduced graphene oxide sheets to create highly stable membranes with engineered nanochannels, demonstrating improved water permeability and enhanced membrane selectivity.⁹⁻¹⁰

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CT20: THz spectroscopy of graphene complementary split ring resonators

Suzuki, Satoru (NTT Basic Research Labs., Atsugi, JPN); Yamamoto, Hideki (NTT Basic Research Labs., Atsugi, JPN)

Split ring resonators are used as a fundamental constituent of metamaterial to obtain negative permeability. Several simulation studies have shown that plasmonic split ring resonators consisting of graphene have excellent performance in the THz region, owing to the relatively long life time of plasmons in graphene [1-3]. In the THz region, the light-graphene interaction is dominated by intraband transition, and absorption can easily exceed the universal absorption of 2.3 %/layer caused by interband transition [4]. Moreover, the optical properties of a graphene split ring resonator, such as the resonance frequency, can be tuned by gate voltage, which can not be achieved in a conventional metal split ring resonator. Nevertheless, to the best of our knowledge, no experiments on graphene split ring resonators have been reported. We fabricated complementary split ring resonators by patterning double-layer graphene grown on a SiC substrate. In the complementary split ring resonator device, the graphene layer has a continuous form. Thus, we can expect that the Fermi level of the entire graphene layer, and thus, the resonance frequency of the device, can be tuned by using an ion liquid- or ion gel-based gating method [5]. The devices showed resonances at about 2.5 and 6.5 THz for x- and y-polarized light, and the absorption was estimated to be about 3 and 6 % at the resonance frequencies, which are comparable or even larger than the interband absorption. The experimentally observed spectra were fairly consistent with simulations. These results show the possibility of graphene-based configurable metamaterials.

This work was partly supported by JSPS KAKENHI.

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CT21: Tuning Thermoelectric Properties of Single Wall Carbon Nanotubes by Electric Double Layer Carrier Injection

Yanagi, Kazuhiro (Tokyo Metropolitan University, Tokyo, JPN); Oshima, Yuki (Tokyo Metropolitan University, Tokyo, JPN); Kitamura, Yoshimasa (Tokyo Metropolitan University, Tokyo, JPN); Nakamura, Masatoshi (Tokyo Metropolitan University, Tokyo, JPN); Kawai, Hideki (Tokyo Metropolitan University, Tokyo, JPN); Maniwa, Yutaka (Tokyo Metropolitan University, Tokyo, JPN)

Thermoelectrics are a very important technology for efficiently converting waste heat into electric power. Hicks and Dresselhaus proposed an important approach to innovate the performance of thermoelectric devices, which involves using one-dimensional materials and properly tuning their Fermi level (PRB 1993). Therefore, understanding the relationship between the thermoelectric performance and the Fermi level of one-dimensional materials is of great importance to maximize their thermoelectric performance. Single wall carbon nanotube (SWCNT) is an ideal model for one-dimensional materials. Previously we reported continuous p-type and n-type control over the Seebeck coefficients of semiconducting SWCNT networks with diameter of 1.4 nm through an electric double layer transistor setup using an ionic liquid as the electrolyte (Yanagi et al, Nano Lett. 14, 6437 2014, Appl. Phys. Lett. 107, 043106 2015). We clarified the thermoelectric properties of semiconducting SWCNTs with diameter of 1.4 nm as a function of Fermi level. In this study, we investigated how the chiralities and electronic structures of SWCNTs influence on the thermoelectric properties. We found the significant difference between the thermoelectric properties of SWCNTs with different electronic structures.

CT22: Asymmetric dye-filled carbon nanotubes for nonlinear optics

Cambré, Sofie (University of Antwerp, Antwerp, BEL); Campo, Jochen (University of Antwerp, Antwerp, BEL); Van Bezouw, Stein (University of Antwerp, Antwerp, BEL); Van Werveke, wouter (University of Antwerp, Antwerp, BEL); Beirnaert, Charlie (University of Antwerp, Antwerp, BEL); C. Verlackt, Christof (University of Antwerp, Antwerp, BEL); Cool, Pegie (University of Antwerp, Antwerp, BEL); Wenseleers, Wim (University of Antwerp, Antwerp, BEL)

Asymmetric dipolar molecules with a large second-order nonlinear optical (NLO) response, find applications in ultrafast electro-optic switches and in wavelength conversion of lasers.¹ In 3D bulk materials, however, such dipolar molecules tend to align in a pairwise anti-parallel way, thus cancelling each other's NLO responses. Here we show that by encapsulating such molecules in the 1D internal channel of single-wall carbon nanotubes (SWCNTs), Coulomb interactions naturally favor a polar head-to-tail alignment, leading to a coherent addition of their second-order NLO responses.² Fluorescence-excitation³ and resonance Raman⁴ experiments evidence the dye-encapsulation. Wavelength-dependent hyper-Rayleigh scattering^{5,6} experiments effectively show that these organic-SWCNT nanohybrids possess giant NLO responses (~50-70 identically aligned dyes). Their equally giant dipole moment and size promises a stable alignment in a polymer film, opening an entirely new route to the rational design of solution-processible yet stable NLO materials. *This work has received funding from the ERC under Horizon 2020 (679841: ORDERin1D) and the FWO-Vlaanderen.*

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POSTER SESSION G: Composites

G1: Carbon nanotube inorganic hybrids for environmental catalysis

Gebhardt, Paul (Technische Universität Wien, Wien, AUT); Dieterle, Dennis (Technische Universität Wien, Wien, AUT); Lukashuk, Liliana (Technische Universität Wien, Wien, AUT); Föttinger, Karin (Technische Universität Wien, Wien, AUT); Rupprechter, Günther (Technische Universität Wien, Wien, AUT); Eder, Dominik (Technische Universität Wien, Wien, AUT)

Recent years saw the introduction of a promising new class of multifunctional materials, nanocarbon-inorganic hybrids, which have a huge potential to overcome limitations of conventional heterogeneous catalysts. In contrast to composites, where a tiny volume fraction of the nanocarbon, e.g. carbon nanotubes (CNTs), is used as a nanostructured filler within an inorganic matrix, hybrids are created by coating the nanocarbons with a thin layer of the functional inorganic material (i.e. semiconductor catalyst). The benefits of this system arise from the close proximity of the two compounds, which enables interfacial charge and energy transfers, as well as morphology effects during material synthesis. Here, we present hybrids of cobalt oxide and vanadium oxide with CNTs. In both cases, the hybridization produced a wide range of morphologies – ranging from coatings with a controlled thickness, over flake-like structures to octahedral, cubic or round nanoparticles of controlled size – depending on the non-covalent functionalization agent and the surface properties of the CNTs. First catalytic results in low-temperature CO and methanol oxidation, for cobalt- and vanadium oxide respectively, revealed beneficial effects of the hybridization, resulting in a significant downshift of minimal reaction temperature. Furthermore, the experiments indicated a clear performance and product selectivity dependence on the phase and particle size of the catalyst, which has to be investigated further in the future. The results were supported by extensive materials characterization, including electron microscopy (TEM, SEM), N₂ physisorption (BET, t-plot, BJH), X-ray diffraction (XRD), thermal analysis (TG/DTA), fourier-transformed infrared spectroscopy (FTIR), Raman spectroscopy, and UV-vis spectroscopy.

G2: Carbon nanotube-grafted carbon fiber composites: damage characterization on the micro-scale

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Carbon nanotubes (CNTs) have excellent mechanical properties and are extremely promising for reinforcement of composites. Multiwall CNTs were directly grown on carbon-fibers by means of chemical vapour deposition (CVD). By using the oxidative

dehydrogenation reaction of C₂H₂ and CO₂, carbon-fiber/CNTs hybrid materials were produced without damaging the carbon-fiber surface. Uni-directional (UD) nano-engineered carbon-fiber reinforced composites (nFRCs) were fabricated using these hybrid materials impregnated with epoxy. The nFRCs were subjected to single fiber push-out tests which showed a 35.7% decrease of the interfacial shear strength (IFSS) compared to the composites without CNTs. By means of in-situ transverse three-point bending tests performed on pre-notched composite beams, the fracturing behaviour was studied parallel to the fibers. In the case of nFRCs containing CNTs, CNTs bridging as well as matrix failure have been observed apart from fiber/matrix debonding. These results demonstrate that the presence of CNTs in nFRCs affects the stress distribution, damage initiation and propagation. With the CNTs grafting, the stress concentration seems to shift from the fiber/matrix interface to CNT/matrix interface.

G3: Room Temperature Electrical and Thermal Switching CNT Composites

Zheng, Ruiting (Beijing Normal University, Beijing, CHN)

Switchable electrical and thermal conductivities are desirable in many applications such as automatic regulation of building temperature, circuit protection, etc. In this paper, we study the electrical and thermal conductivities of multi-walled carbon nanotubes (MWCNTs) composites via first order phase transition. Surface functionalization of MWCNTs plays a vital role for the re-dispersion and transport properties of the composites. We demonstrate that, with different base fluids, the composites show electrical switching and thermal switching properties at different temperature. Around the phase transition point, the corresponding contrast ratio of electrical and thermal conductivities reaches 5 orders and 3.58 times respectively.

G4: A novel strategy to fabricate Co-MWCNTs hybrids: Influence of MWCNT nature on the hybrid formation

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MWCNTs, filled with metals, can be used for various applications in nanotechnology, biomedical sciences, memory device technology, and in catalysis. In the present work, the influence of the MWCNT nature was investigated on the features of Co-MWCNT hybrids formation. MWCNTs were synthesized by CVD method of ethylene decomposition over the bimetallic Fe-Co catalysts with different metal loadings and various supports at 680°C (the surface area of MWCNT was 115-380 m²/g, the average particle diameter of 7.2-18.6 nm). An important step of the hybrid preparation is the creation of the anchoring sites for Co on the MWCNTs surface. To achieve that, functionalized MWCNTs containing surface carboxylic groups (ca. 0.8 groups per 1 nm²) were produced by the treatment with boiling concentrated nitric

acid. Co-containing samples were prepared by the impregnation of as synthesized and functionalized MWCNTs with the aqueous solutions of Co (II) salts followed by calcination under an Ar atmosphere and reduction in H₂ flow at 350°C. The samples with Co content of 5-20 wt.% on the different types of MWCNTs were obtained. For the investigation of the structure and morphology of Co-containing MWCNTs, TEM, XRD, IF ⁵⁹Co NMR methods were used. The all samples with Co content up to 10 wt.% mainly contain Co particles within the channels of MWCNTs. Co particles inside the channels of MWCNTs with average diameter of 7.2 and 9.4 nm have rounded shape and the average diameter of 3-5 nm, which is determined by the internal diameter of the channels. The samples produced using MWCNTs with an average diameter of 18.6 nm contain elongated Co particles of more than 100 nm inside the MWCNTs. MWCNTs modification by Co metal nanoparticles can potentially alter the dielectric and magnetic permeability of the MWCNTs thus making Co/MWCNT hybrids a new material for electro-magnetic applications such as radiofrequency shielding.

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G5: Anisotropic Magnetic Properties of an Endohedral Metallofullerene Ce@C82 for Molecular Location Sensing

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Recently, our group has reported anisotropic magnetism of an endohedral metallofullerene Ce@C82 both in a pristine form and chemically functionalized form [1,2]. Remarkably, the anisotropy of the magnetism which is led by the encapsulated Ce atom was slightly influenced by the carbene addition reaction. In addition, absolute position of the hydrogen atoms of the addend was assigned by the difference in the effective distance of the anisotropic magnetism, which is decreased with the cube of distance between the Ce and hydrogen atoms. In this presentation, we present a novel molecular location sensing method based on an endohedral metallofullerene, Ce@C82, using its anisotropic magnetic properties which lead to temperature-dependent paramagnetic shifts in ¹H-NMR spectra [3]. The strong stability and low toxicity of encapsulated Ce@C82 makes it a suitable candidate for molecular location probes in harsh conditions in material science and biological systems. To achieve this concept, five site-isomers of Ce@C82CH₂-3,5-C₆H₃Me₂ were chemically synthesized by a radical coupling reaction [4] and characterized by means of a crystal structure, absorption spectra and density functional theory calculations. The temperature-dependent shifts in ¹H-NMR spectra of the isomers, which are induced by the magnetic anisotropy of the caged Ce, were correlated to the distance and relative position of the proton from the Ce atom. Detailed numerical analysis of the shifts using suitable criteria successfully located the relative position of the nearby hydrogen atoms from the inside Ce atom. These results evidenced that the

paramagnetic shifts based on the anisotropic magnetism of the encapsulated Ce atom can be used for molecular location recognition.

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- [3] Y. Takano et al., submitted.
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G6: Carbon nanotube/polymer nanofibers prepared by laser-heated electrospinning

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A laser-heated electrospinning for obtaining the mechanically strong multi-walled carbon nanotubes (MWNTs)/poly(ethylene terephthalate) (PET) nanofibers is demonstrated using a near-infrared laser irradiation. The laser was irradiated just below the spinneret of polymer fluid jet stream during the electrospinning. The orientation factors of MWNT and PET chain for the laser-heated electrospun nanofibers were measured using a polarized Raman spectroscopy. It was found that the laser-heated electrospun fibers showed high orientation of MWNT and PET chains, whereas the electrospun nanofibers without laser heating showed low orientation of MWNTs and PET chains. The orientation of MWNT in the laser-heated electrospun nanofibers was better developed than orientation of PET chains. The mechanical properties of the laser-heated electrospun PET/MWNT nanofibers were also largely enhanced, compared to those of electrospun nanofibers without laser heating. Dependence of breaking stress and modulus on the laser power density was corresponded well to dependence of MWNT orientation on the laser power density. It is concluded that the laser-heated electrospinning in this study is a very effective method for enhancing the MWNT alignment and resultant mechanical properties of nanofibers.

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G7: Fabrication and electrical properties of carbon nanotube-copper composite wires

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Carbon nanotube-copper composites (CNT-Cu) have demonstrated high electrical and thermal conductivities at par with Cu, low coefficients of thermal expansion similar to Si, and current carrying capacities exceeding that of Cu [1-3]. In combination with low densities, CNT-Cu is a promising candidate for applications

requiring low-weight high-performance materials. Our group has previously reported the production of CNT-Cu composites as sheets and microfabricated patterns [1-3]. However, to spur industrial application of CNT-Cu, fabricating the composites in the form of wires is vital. Macroscopic high-performance CNT-Cu wires can potentially address the rising demand for lightweight conductors in smart fabrics, motor windings, electrical wiring, etc. Here, we report for the first time the production of fully filled CNT-Cu wires by two-stage electrodeposition of CNT wires. In our CNT-Cu wires, the Cu (96-98 wt%) is uniformly distributed throughout the CNT matrix. Complete uniform Cu filling is crucial for the composite to reflect the combinatorial properties of CNTs and Cu. We will discuss the effect of various process parameters, such as the electrodeposition current, time, environment, solution concentration, etc. on the filling and internal structure of the wires. We will also present the electrical properties of the CNT-Cu wires. This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

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[3] C. Subramaniam et al. Nanoscale 8, 3888 (2016).

G7: Graphene and water-based elastomers ultra-thin-film composites

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Elastomers are viscoelastic polymers with weak inter-molecular forces that exist in an amorphous state above their glass transition temperature. Elastomers can be classified as thermosets or thermoplastics. The most common thermoset elastomer is vulcanized natural rubber latex (NRL), which is most commonly processed in the form of a latex, a stable dispersion (emulsion) of polymer microparticles in an aqueous medium. Also common are thermoplastic polyurethanes (PU), in this case an anionic aliphatic polyester polyurethane dispersion in water. We demonstrate composites with both graphene oxide and reduced graphene oxide, the reduction being undertaken in-situ or ex-situ using a biocompatible reducing agent in ascorbic acid. The graphene/wPU composite incorporates graphene flakes in between polymer chains, whereas the graphene/NRL composite incorporates the graphene in between polymer microparticles. The ultrathin films were cast by dip molding. The transparency of the elastomer films allows us to use optical microscopy image and confirm the uniform distribution as well as the conformation of the graphene flakes within the composite. We show that graphene can be used to reinforce 20 micron thin elastomer films, resulting in over 50% increase in elastic modulus at a very low loading of 0.2 wt%, while also increasing the elongation to failure. This loading is below the percolation threshold for electrical conductivity. Thin-film elastomers (elastic polymers) have a number of technologically significant applications ranging from sportswear to medical devices.

G9: Graphene Nanoribbons supporting Pt nanoparticles composites for catalytic reduction of 4-nitrophenol to 4-aminophenol

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Wang, Shan-Yu (National Taiwan University of Science and Technology, Taipei, TWN);

Chiang, Wei-Hung (National Taiwan University of Science and Technology, Taipei, TWN)

Graphene nanoribbon (GNR) represents a unique form of carbon materials and have spurred intensive interests due to their exceptional electronic property, thermal stability, and low percolation threshold. Recent theoretical and experimental works demonstrated that GNRs are promising materials for many applications such as energy generation and storage, chemical and biosensors, catalysis, nanocomposites, and nanoelectronics. To further boost the advantages of GNRs, metal nanoparticles (NPs) were selected to form various types of composite material for plenty applications including, energy storage, photocatalyst, electrochemical sensors, and especially catalysis. The unique nature of GNR-NP composite materials with high surface area and exceptional conductivity can assist the chemical reaction to lower the activation energy and increase reaction rate constant. Here we report a facile synthesis of GNR-PtNP composites as a green catalyst for catalytic reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP). 4-NP has been a persistent wastewater constituent from various industries. Consequently, a catalytic method is sought-after in reducing 4-NP to less toxic and commercially important 4-AP. GNR was prepared by an intercalation-assisted longitudinal unzipping of single-walled carbon nanotubes (SWCNTs). KNO_3 was used as intercalation agent that weaken Van der Waals attraction between CNT walls to facilitate the GNR formation. The process generated oxygen-containing groups on the GNR surface, providing the anchoring site for Pt-NPs nucleation and growth via a wet-chemical reaction. Detailed materials characterizations and systematic catalysis study indicate that GNR-PtNP composites show superior catalytic performance with a normalized reaction rate constant (k_n) of $120 \times 10^{-3} \text{ mmol}\cdot\text{s}^{-1}\cdot\text{g}^{-1}$. Our work suggests that GNR-PtNP composite materials show a great potential to develop an effective and stable catalyst for environmental protection.

G10: Highly Selective Purification of Metal Impurities from MWCNTs and Preparation of MWCNT/EEA Composites for High-voltage Cables

Hyun, Yesub (Sejong University, Seoul, KOR)

A high-voltage cable typically consists of the conductor, inner semiconducting layer, insulation layer, outer semiconducting layer, metal screen layer, and sheath. The semiconducting layers protect the insulation layer from breakdown by filling air gaps between the conductor and insulation layer as well as distributing uniformly electric fields over the insulation. The semiconducting layer are commonly composed of polymer such as ethylene ethyl acrylate (EEA) and carbon fillers such as carbon black (CB) and carbon nanotubes (CNTs). CNTs are preferred to CB due to their low loading amount. However, a high content of metal catalysts in CNTs may induce breakdown of the cable by forming electrical trees in the insulation layer so that it is

essential to use highly pure CNTs for this application. Our previous study showed that metal catalysts encapsulated by graphitic layers were hardly removed by the gas-phase purification using chloroform. This study first decapsulated the graphitic layers to expose the metal catalysts inside them by introducing water vapor into the quartz tube at 500 ° C. Our multi-walled CNTs were synthesized using Al₂O₃ and MgO support embedded with Fe and Co catalysts. The Al₂O₃ and MgO in the CNTs were easily removed by refluxing HCl, and the Fe and Co were effectively purified at 800 ° C using bubbled chloroform. Finally we obtained highly pure CNTs having the metal content as low as 100ppm from the raw CNTs with the 5,130-ppm metallic impurities. The composites were prepared by dispersing separately EEA and CNTs in xylene and by mixing them together under mechanical stirring. This solution was added to ethyl alcohol to precipitate the solid MWCNT/EEA. The solid mixture was dried in oven, mixed with cross-linking agent and pressed at 180 ° C, producing a thin composite sheet. We prepared the sheets using CNTs of every purification step and then characterized their electrical resistivities, which varied depending on the surface states of CNTs.

G11: High-performance multi-functional reverse osmosis membranes obtained by MWCNT/PA nanocomposite

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Clean water obtained by desalinating sea water or by purifying wastewater, constitutes a major technological objective in the so-called water century. In this work, a high-performance reverse osmosis (RO) composite thin membrane using multi-walled carbon nanotubes (MWCNT) and aromatic polyamide (PA), was successfully prepared by interfacial polymerization. The effect of MWCNT on the chlorine resistance, antifouling and desalination performances of the nanocomposite membranes were studied. We found that a suitable amount of MWCNT in PA, 15.5 wt.%, not only improves the membrane performance in terms of flow and antifouling, but also inhibits the chlorine degradation on these membranes. Therefore, the present results clearly establish a solid foundation towards more efficient large-scale water desalination and other water treatment processes.

G12: Microwave Induced Welding of Carbon Nanotube-Thermoplastic Interfaces for Enhanced Mechanical Strength of 3D-Printed Parts

Sweeney, Charles (Texas A&M University, College Station, USA); Saed, Mohammad (Texas Tech University, Lubbock, USA); Green, Micah (Texas A&M University, College Station, USA)

Three-dimensional (3D) printed parts produced by fused-filament fabrication of a thermoplastic polymer have become increasingly popular at both the commercial and consumer level. The mechanical integrity of these rapid-prototyped parts however, is severely limited by the inter-filament bond strength between adjacent extruded layers. In this report we propose for the first time a method for welding thermoplastic interfaces of 3D printed parts using the extreme heating response of multi-walled carbon nanotubes (MWCNTs) to microwave energy. To achieve this, we developed a coaxial printer filament with a pure polylactide (PLA) core and a CNT composite sheath. This produces parts with a thin electrically percolating network of MWCNTs at the interfaces between adjacent extruded layers. These interfaces are then welded together upon microwave irradiation at 2.45 GHz. Our results indicate that the tensile strength of the interface can be restored to values approaching that of the bulk polymer. We also investigated the dielectric properties of PLA/MWCNT composite films at microwave frequencies and performed in-situ microwave thermometry using a forward-looking infrared camera to characterize the heating response of the composites upon microwave irradiation.

G13: Novel Functionalization method of well aligned Carbon Nanotube and their polymer composite properties

Moon, Sook Young (Japan Aerospace Exploration Agency, Mitaka, JPN)

Carbon nanotubes (CNTs) have been considered for many applications because of their extraordinary physical, chemical, and mechanical properties. Despite their many desirable properties, the hydrophobicity and chemical inertness of CNTs hinders their commercial utilization. To overcome these limitations, CNT surfaces were functionalized using either covalent (chemisorption) or non-covalent modification (physisorption). Covalent surface modification involves the direct incorporation of new elements or organic functionalities into the CNT sidewalls. But a major problem of both chemical and physical surface modifications remained the impurity onto the CNT surface and some impurity is difficult to remove in further processes or applications. Therefore, development of a better and more effective functionalization method remains a major challenge. In this study, we report a novel method to modify CNT surfaces and developed composite with epoxy resin. This method has been proven to be effective in terms of making functionalized CNT surface and improving interaction between CNT and polymer without braking alignment. Interactions between surface properties of the CNT and mechanical properties are discussed in relation to the treatment conditions.

G14: Single walled carbon nanotube based melt-mixed polymer composites for thermoelectric applications

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Electrically conductive polymer composites (CPCs) are well developed for diverse applications, such as dissipation of static electricity. Carbon nanotubes (CNTs) with their high electrical conductivity are intensively employed to fabricate CPCs. At the same time, the thermal conductivity of such composite remains low due to the intrinsic low thermal conductivity of polymer. Therefore, CPCs filled with CNTs are also studied as potential thermoelectric materials (high electrical conductivity, high Seebeck coefficient and low thermal conductivity) to recover waste heat into electric energy. Low cost production techniques such as solution or melt processing are typically used to fabricate CPCs. Melt processing, compared to solution mixing, avoids solvents and can be easily scaled up to industrial level. In our study, composites with an industrially widely used polymer, namely polypropylene (PP) as the matrix were prepared by melt processing. Single walled carbon nanotubes were used to construct an electrical conducting network, in which electrical percolation occurs already at 0.2 wt% CNTs. The charge carriers injected by CNT addition are however detrimental to the Seebeck coefficient. On the other hand, the addition of ionic liquid (IL) together with CNTs, simultaneously increases the electrical conductivity and Seebeck coefficient compared to composites filled with only CNTs. The highest obtained Seebeck coefficient of such melt prepared composites with mixed filler system is about 63 $\mu\text{V}/\text{K}$, much larger than that common solution processed conjugated polymers, e.g. PEDOT:PSS (ca. 20 $\mu\text{V}/\text{K}$). The effectivity of this mixed filler system of CNTs and IL inside PP matrix is dependent on the CNT types. In addition, it is intended to develop both n-type and p-type composites from the same base material for better compatibility regarding device fabrication.

G15: Stabilizing active edge sites in Semi-Crystalline Molybdenum Sulfide by anchorage on Nitrogen-Doped Carbon Nanotubes for Hydrogen Evolution Reaction

Ekspong, Joakim (Umeå University, Department of Physics, Umeå, SWE)

Finding an abundant and cost effective electrocatalyst for the hydrogen evolution reaction (HER) is crucial for a global production of hydrogen from water electrolysis. In this work, we report of an exceptionally large surface area hybrid catalyst electrode comprising semi-crystalline molybdenum sulfide (MoS_{2+x}) catalyst attached on a

substrate based on nitrogen-doped carbon nanotubes (N-CNT), which are directly grown on carbon fiber paper (CP). We show that nitrogen-doping of the carbon nanotubes improve the anchoring of MoS_{2+x} catalyst compared to undoped carbon nanotubes and concurrently stabilizes a semi-crystalline structure of MoS_{2+x} with a high exposure of active sites for HER. The well-connected constituents of the hybrid catalyst are shown to facilitate electron transport and as a result of the good attributes, the $\text{MoS}_{2+x}/\text{N-CNT}/\text{CP}$ electrode exhibits an onset potential of -135 mV for HER in 0.5 M H_2SO_4 , a Tafel slope of 36 mV dec^{-1} and high stability at a current density of -10 mA cm^{-2} .

G16: Synergy Effect of Nanocarbon and Boron Nitride as Filler Materials in Thermally Conductive Nanocomposites

Agustina, Elyse (Sejong University, Seoul, KOR)

Nanocarbon materials, renowned for their outstanding thermal properties, have been greatly considered to be applied to heat sinks of electronic devices. Among many heat sink materials, polymer composites containing thermally conductive fillers are favorable due to their low weights, low prices, high chemical resistance, and easy processability. This study first investigated synergy effect of two different nanocarbon materials, exfoliated graphite (EG) and carbon nanotubes (CNTs), on thermal, electrical, and mechanical properties of the polymer composites. These hybrid fillers were incorporated into the polymer matrix in the range of 0.5-20 wt.%. Interestingly, the synergy effect of the hybrid fillers was maximized at the EG/CNT ratio of 6:4 for the low filler loading of 0.5 wt.% and at the ratio of 9.7: 0.3 for the filler content higher than 2 wt.%. The synergistic improvement mechanism was proposed by observing the distribution of EG and CNTs in the matrix with SEM and optical microscope. We studied further the synergy effect of the third filler by adding boron nitride (BN) to the nanocomposites containing EG and CNTs. BN was designed to replace partly EG in the composites as it possesses the same multilayered platelet shape as graphite. In the three-filler composites, the synergy effect of BN on thermal and mechanical properties occurred at $(\text{EG}_{0.9}\text{BN}_{0.1})_{0.97}\text{CNT}_{0.03}$ composition for 10 wt.% loading. A suitable filler alignment model would be suggested to explain the synergistic hybridization of three fillers in the nanocomposites. The composite samples were prepared via a solvent-assisted process where the fillers were dispersed by sonication for 2 h at 500 W. Thermal conductivities, tensile strengths, and electrical resistances were measured using laser flash system, ultimate tensile machine, and two-probe method, respectively.

POSTER SESSION H: Theory and Simulation

H1: Electronic states of collapsed carbon nanotubes: Displaced bilayer graphene with closed edges

Nakanishi, Takeshi (AIST, Tsukuba, JPN); Ando, Tsuneya (Department of Physics, Tokyo Institute of Technology, Tokyo, JPN)

Band structure is theoretically studied in collapsed zigzag and armchair nanotubes within an effective-mass scheme[1]. The collapsed tubes are regarded as ribbons of bilayer graphene with closed edges described by boundary conditions explicitly derived. Within the effective-mass scheme, effects of inter-wall interactions are shown to be important in non-chiral nanotubes such as zigzag and armchair. In fact, with the increase in the width of the flattened region, the band structure approaches that of a bilayer ribbon in which the electron motion in the ribbon-width direction is discretized. The same results can be derived by calculating boundary conditions corresponding to the closed-edge structure in which the top and bottom layers are smoothly connected through a monolayer graphene. Effects of the closed-edge are shown, including band gap opening for the bilayer graphene in AB stacking, and chiral states, when armchair nanotubes are collapsed into AA or AA' stackings. [1] T. Nakanishi and T. Ando, Phys. Rev. **B 91** (2015) 155420.

H2: First-principles molecular dynamics simulations for graphene growth mechanism on SiC surface - Growth process from 1D carbon chains to 2D graphene sheets

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An epitaxial graphene sheet can be obtained by heat sublimation of Si atoms from the SiC surface. However its growth mechanism is yet not understood in detail. The aim of this study is to understand this mechanism at the atomic-scale by first-principles molecular dynamics (FPMD) simulations. A first-principles calculation code PHASE/o which is appropriate for efficient large scale parallel calculations is used. Before starting the MD, some of the Si atoms on the top layer are intentionally removed from the initial SiC substrate to emulate the Si heat sublimation. Then, MD is executed for 1 psec. and after this, the whole system is relaxed. This set of procedures (i.e. 'Si removal', '1 psec. MD', and 'relaxing') is repeated for three times. Using the structure obtained after such preliminary series of simulations, next we executed main MD for about 10 psec. and tracked the behavior of the redundant C atoms. The result gives us a new perspective on the growth mechanism in which a number of C-chains are formed on the SiC surface and consequently become a part of graphene-like 2D-structures. The graphene growth mechanism proceeds as follows. A number of 1D C-chains are formed and start to extend from a very early stage of the MD. They can easily diffuse since only one or both ends are bonded to the surface, and some of them gather with each other to make C-rings. Some of such C-rings

stand stably on the (0001) terrace supported by the Si atoms below. This will be an initial base of a new graphene sheet and it starts to grow by absorbing other C-chains surrounding it. We are going to have a detailed discussion about where, when and how do these C-chains be formed and finally become 2D-structures. A portion of this research was supported by the grant from MEXT's project and carried out in partnership with the University of Tokyo. K computer is used for the simulations.

H3: Highly Efficient Thermo-acoustic Ultrasound Transducer with Carbon Nanotube Film

Kim, Duckjong (Korea Institute of Machinery and Materials, Daejeon, KOR); Moon, Choongman (Center for Advanced Meta-Materials, Daejeon, KOR); Ha, Kang Lyeol (Pukyong National University, Busan, AUT)

Thermo-acoustic effect driven by pulse laser heating can generate ultrasound with very high amplitude and frequency, and it makes the thermo-acoustic ultrasound transducer a promising candidate for replacing the conventional piezoelectric ultrasound transducer. However, low energy conversion efficiency has been a serious drawback in practical use of the thermo-acoustic ultrasound transducer. In this study, we build a simulation model and obtain analytical solutions for thermo-acoustic ultrasound generation, which are in good agreement with experimental results for ultrasound transducers with carbon nanotube film. By using the analytical solutions, we discuss how to improve the energy conversion efficiency of the transducer. Our results show that damping reduction and resonance could be important solutions for efficiency improvement.

H4: Molecular Dynamics Simulation of Chirality-Defined Carbon Nanotubes Growth

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Molecular dynamics (MD) simulations are often used to analyze the mechanism of carbon nanotube (CNT) growth¹. However, because CNTs grown in MD simulations were too defective, the mechanism of chirality-selection is almost never discussed despite experimental reports of chirality specific growth². We have successfully simulated several kinds of chirality-defined nanotube growth on Co and Fe catalyst by tuning the temperature and the free (gas phase) carbon density. In addition, we developed Tersoff-type potential of bimetallic catalysts including Fe-Co, Cu-Co and W-Co. The chirality of nanotubes grown from these bimetallic catalysts in simulation will be discussed as well.

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[2] F. Yang, et al., Nature, 510 (2014) 522.

H5: Polyynes Electronic and Vibrational Properties under Environmental Interactions

Wanko, Marius (University of the Basque Country, San Sebastian, ESP); Rubio, Angel (MPI for the Structure and Dynamics of Matter, Hamburg, GER); Pichler, Thomas (University of Vienna, Wien, AUT)

Recent advances allow growing linear carbon chains of up to thousands of atoms inside carbon nanotubes [1]. This increases the interest in the unique properties of carbyne and finite polyynes and their response to different environments. Here, the experimental characterization still relies on empirical or bulk-physical models appropriate for specific chain lengths or environments. The physical understanding of the observed trends in terms of charge transfer, electron delocalization, and van-der-Waals interactions is widely missing. In this contribution, we theoretically describe the main interactions between polyynes and graphene or carbon nanotubes and develop models that better account for the experimental conditions and can be applied to physisorbed molecules in general. [1] L. Shi et al., , DOI: 10.1038/NMAT4617

H6: Ab initio calculation of optical spectra of strained carbon nanotubes

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Carbon nanotube (CNT) optics is an active field of research and is becoming increasingly interesting for applications. CNTs show unique properties upon strain: Under load, their band gap is opening or closing (depending on the CNTs' chirality) which makes them suitable for electronic and optical strain sensing at the nano scale. Further, they could operate as strain-tunable emitters. Our theoretical investigations of strained CNTs show strongly bound excitons that drastically modify the optical spectrum of CNTs with respect to single-particle pictures. The resulting optical transitions strongly shift with respect to strain. However, the shift of the optical transition differs from the shift of the corresponding electronic state. Additionally, the strain-dependent, intrinsic carrier screening alters the exciton binding energy. Higher optical transitions, depending on their order, shift either in the same or in the opposite direction compared to the first one. This behavior originates from the shift of electronic bands, which can be qualitatively understood by the tight-binding zone folding scheme. Quantitatively, the exciton binding strength decreases again, as the strain increases. For example the second optical transition of the (8,0)-CNT shifts through the entire visible spectral range if strained by a few percent. For our calculations, we use independent-particle (density functional theory, DFT) and single-quasiparticle band structures (GoWo@LDA) to investigate the strain-dependence of the band gap. Further, the Bethe-Salpeter equation is applied for the calculation of the optical spectra in order to describe excitonic effects. In a one-dimensional system, these calculations require the truncations of the Coulomb interaction between periodic images in the supercell approach. The parameters obtained by these calculations can be used for optical device modeling based on strained CNTs as well as CNT spectroscopy, e.g. infrared spectroscopy, and may allow an extrapolation to other CNTs.

H7: An Atomistic Model for Carbon Nanotube Based Field-effect Transistors: Interband Tunneling and Device Scaling

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We study carbon nanotube based field-effect transistors (CNTFETs) consisting of n-doped source and drain electrodes together with an ideal wrap-around gate. This system is comparable to the one studied experimentally by Lu et al.¹ and is our model for comparing different simulation approaches. In this contribution, we present our results based on a fully atomistic quantum transport model. Carbon nanotubes (CNTs) with diameters ranging from 0.5 nm to 1.3 nm, which corresponds to the (7,0) CNT and (16,0) CNT, respectively, are studied. We find that in case of thick CNTs, the band-to-band tunneling (BTBT) strongly increases the leakage current in the off-state. This leads to ambipolar transfer characteristics in agreement with experimental results¹. Concerning very thin CNTs, the BTBT has not been studied in much detail, yet. We demonstrate that for these kind of CNTs, states within the channel are strongly localized. They do not allow carrier transport and thus suppress the BTBT, which results in ideal unipolar transfer characteristics and on/off ratios of about 10⁷. We furthermore present a systematic investigation of the relation between device parameters and the resulting transistor characteristics, which can guide future device scaling. Thin CNTs for example allow outstanding device properties even for short channel lengths down to 8 nm. It is crucial to maintain channel control in ultra-scaled transistors. Thus, our studies also elucidate the impact of aggressive gate scaling. Even for a very small gate electrode of only 0.4 nm length, good switching properties can be preserved. The non-equilibrium Green's functions formalism together with self-consistent extended Hückel theory is used for the simulations. Thanks to a parameter set previously developed in our group², we can describe CNTs with a density functional theory-like accuracy. ¹Lu et al., *Journal of the American Chemical Society* **128** (2006) ²Zienert et al., *Nanotechnology* **25** (2014)

H8: Analysis of size effects in interaction of carbon nanotubes with functionalized gold nanoparticles. A molecular dynamics study.

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Among many applications of carbon nanotubes (CNTs) the area of nanomedicine and drug delivery is being explored extensively. Various anticancer drugs were used in conjunction with CNTs forming covalently or noncovalently bonded compound. Noncovalent attachment allows for large loadings and does not alter the chemical nature of drug molecules. At the same time the binding is relatively weak and thus leaking of drugs may occur. Deposition of colloid nanoparticles on surfaces of CNTs leads to creation of hybrid materials with unique properties, i.e. colloidal nanoparticles are frequently analysed as modifiers of CNTs. Carbon nanotubes are

particularly useful as carriers of platinum based drugs . Often, the drugs are encapsulated in the inner cavity of nanotubes and are locked by some removable caps placed at the nanotube tips. The studied system is composed of a carbon nanotube and two gold nanoparticles covalently linked to the nanotube tips by fragments containing hydrazone bonds . The aim of this study is the analysis of how various modifications of CNT and gold nanoparticles sizes affect the dispersion forces between these two compounds. Keeping these forces in optimal range is crucial for construction of a system which upon cleavage of covalent linkers allows for spontaneous uncapping/recapping of the nanotube tips .

H9: Angular momentum and topology in finite-length single-wall carbon nanotubes

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Recent studies of quantum transport have revealed that single-wall carbon nanotubes (SWNTs) contain richer phenomena, especially in terms of spin and valley. Fourfold degeneracy of discrete energy levels has been considered as an intrinsic property in finite-length SWNTs reflecting the two spin states and the two valley states. Measurements for ultraclean SWNTs show lift of fourfold degeneracy caused by the spin-orbit interaction. Recent studies focused on angular momenta of two valleys in metallic SWNTs, to discuss the valley coupling as another mechanism of lift of degeneracy [1]. For the SWNTs in which two valleys have different angular momenta, the two valleys are decoupled and the spin-orbit interaction lifts the fourfold degeneracy in finite-length. On the other hand, for the SWNTs in which two valleys have the same angular momentum, the valley coupling lifts the fourfold degeneracy. Here we will focus on the semiconducting SWNTs and show that they are classified by means of angular momentum with an integer $d=\text{gcd}(n,m)$, the greatest common divisor of two integers n and m specifying the chirality of nanotubes [2]. It is shown that the valley coupling occurs in the majority (82 %) of SWNTs, *even for ultraclean nanotubes with clean edges*, which conserve the angular momentum of bulk electronic states. In order to explain the valley coupling, an effective one-dimensional lattice model is derived and analyzed. By expanding the theory of valley coupling, a bulk-edge correspondence, relationship between the number of edge states in the energy gap and the topological winding number given in the corresponding bulk system, is derived, which reveals another feature of SWNTs as topological insulating materials. The number of edge states depends not only on the chirality but also on the shape of boundary.

[1] W. Izumida *et al.*, Phys. Rev. B **91**, 235442 (2015).

[2] W. Izumida *et al.*, arXiv:1603.06333

H10: Blocking transport resonances via Kondo many-body entanglement in quantum dots

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Many-body entanglement is at the heart of the Kondo effect, which has its hallmark in quantum dots as a zero-bias conductance peak at low temperatures. It signals the emergence of a conducting singlet state formed by a localized dot degree of freedom and conduction electrons. Carbon nanotubes offer the possibility to study the emergence of the Kondo entanglement by tuning many-body correlations with a gate voltage. Here we quantitatively show an undiscovered side of Kondo correlations, which counterintuitively block conduction channels: inelastic cotunneling lines in the magnetospectrum of a carbon nanotube strikingly disappear when tuning the gate voltage. Considering the global $SU(2) \otimes SU(2)$ symmetry of a carbon nanotube coupled to leads, we find that only resonances involving flips of the Kramers pseudospins, associated to this symmetry, are observed below the Kondo temperature. Our results demonstrate the robust formation of entangled many-body states with no net pseudospin.

H11: Coexistence of Dirac Cone and Kagome Band in Two-Dimensional Network of Hydrocarbon Molecules

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Graphene with periodic porous is known to possess peculiar electronic structure near the Fermi level depending on their π network topology. Polymerization or cyclodehydrogenation of hydrocarbon molecules is the practical procedure to realize such porous graphitic materials exhibiting unusual electronic properties that are tunable by assembling the appropriate hydrocarbon molecules. Phenalenyl molecule ($C_{13}H_9$) possesses radical spin electron owing to non-bonding π electron, so that 2D covalent networks consisting of phenalenyl may exhibit long-range spin ordering among the radical spins localized on each molecule. In this work, we study geometric and electronic structures of 2D networks of copolymer of phenalenyl and phenyl molecules. Our first-principle calculations based on density functional theory with generalized gradient approximation show that a 2D network with planar conformation has both Dirac cone and Kagome band at and just below the Fermi level, respectively, because phenalenyl forms a hexagonal and phenyl forms a Kagome π networks. We also found that the radical spins localized on phenalenyl are antiferromagnetically and ferromagnetically aligned. Among these three states, the antiferromagnetic state is the ground state whose energy is lower than ferromagnetic and metallic states by 14 and 313 meV per cell, respectively.

H12: Electron transport in defective metallic and semiconducting carbon nanotubes

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The electron transport in arbitrary carbon nanotubes (CNTs) with randomly positioned defects is described by a new and very efficient simulation approach. Based on this approach we are able to handle CNTs of realistic size up to several microns with up to thousands of defects. From our model calculations, simple analytic expressions are derived to express the conductivity of CNTs featuring arbitrary defect mixtures. While most of the theoretical studies deal with ideal CNTs, even under best laboratory conditions, defects are introduced to the CNTs during any step of the device fabrication. It is of big interest to know how different defects affect the electronic transport properties of CNTs. We treat this task from a theoretical point of view. The difficulty is the huge number of atoms of defective systems. This makes the usage of density functional theory (DFT), which scales cubically with the number of atoms, unpractical. The transport calculations are based on a fast, linearly scaling recursive Green's function formalism, allowing us to treat large systems quantum-mechanically. The electronic structure is described by a hybrid model which uses the fastness of the tight binding approach as well as the good accuracy of DFT. In our study we focus on mono- and divacancies, which are the most common defects. However, our approach can be extended easily to cover arbitrary defect types. In [1] transmission spectra of metallic CNTs with many defects are studied comprehensively and diameter-dependent localization lengths are extracted. We extend this work to defect mixtures and show that the total localization length can be expressed by those of CNTs with one defect type. Based thereon, we show how to estimate or even predict the conductance of arbitrary defective CNTs. Finally, we focus on defective semiconducting CNTs and show the influence of the structural parameters and the temperature.

[1] F. Teichert et al., New J. of Phys. 16 (2014) 123026

H13: Electronic Structure of Carbon Nanotubes under the Metal Contacts

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Fascinating mechanical and electrical properties of Carbon nanotubes (CNTs), have attracted a lot of attention in recent years. One of the most important applications is CNT field-effect transistors (CNFETs). However, there are challenges left in current devices, while scalability of the CNFET channel has already been shown to sub-10 nm, yielding ballistic transport and device performance that is limited by the resistance at contacts. In CNFETs, typically part of the nanotube is covered by a metal contact. It has been predicted [1,2] that capillary and van der Waals forces cause the nanotube to deform or even collapse under the metal. These deformations can significantly affect the electronic structure (and thus contact resistance), yet to be

investigated. In this paper we are investigating electronic structure and implications for transport properties of CNTs under the metal contacts. In order to calculate the electronic structure of deformed CNTs, we perform atomistic relaxation of carbon atoms in CNTs under the metal extending the previous continuous model calculations. In the modified model, metal and substrate are treated as continuum, as before. The atomic positions of carbon atoms and metal contact geometry is found by minimizing the total energy of the system, and is used to calculate the band structure using Density Functional Theory (DFT). We find striking changes on the band structure, which we understand using a sigma-pi tight binding hamiltonian. The latter allows us to investigate point contact resistance at the round/deformed CNT interface.

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H14: Energetics and electronic structures of GaN thin films

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Two-dimensional (2D) materials with an atom thickness exhibit peculiar properties arising from the constituent elements and network topologies that allow them being a promising material in the wide areas of the future nanotechnology. Following the discovery of graphene, many layered materials, such as h-BN, silicene, MoS₂, and phosphorene, have been synthesized by using various experimental techniques. GaN is a wide band gap semiconductor with excellent optical and electrical properties, which are applicable as optical and high frequency electronic devices because of their high carrier mobility and wide direct band gap. In the present work, we aim to explore the possibility of the 2D network of GaN by analogy with h-BN as the other candidate of the III-V atomic layer materials, using the density functional theory (DFT) by combining with the effective screening medium (ESM) method. Our DFT calculations showed that the GaN thin films with (0001) surfaces and five or less atomic layers prefer layered structure of which band gap sensitively depend on the number of stacked layers. For the monolayer GaN sheet, the sheet is a semiconductor with an indirect band gap of 2.28 eV between the Γ point and K point for the conduction band bottom and valance band top, respectively, under an equilibrium lattice constant of 0.32 nm. We also found that the GaN sheet form a multilayered structure with the interlayer spacing of about 0.22 nm and the binding energy of 0.85 eV. With increasing the number of layers, the valence band top approaches the Γ point. Finally, the multilayer GaN sheet is a direct gap semiconductor with a band gap of 2.78 eV at the Γ oint, which is narrower than that of the 3D GaN with the Wurtzite structure. These results indicate the possibility of band structure modulation of layered GaN with variable layer numbers.

H15: Exciton-Plasmon Coupling and Photonic Band Structure of Carbon Nanotube Arrays

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Carbon Nanotubes (CNs) have unique response properties that can be dramatically changed simply by tuning their chirality and tube diameters. This allows for the possibility of coupling different types of excitations in individual carbon nanotubes. For example, individual CNs are known to support both excitons and interband plasmons, which can be coupled in a controllable way to give rise to a variety of new phenomena and applications [1-3]. If the carbon nanotubes are aligned in a periodic array, excitons and interband plasmons in different tubes couple with each other. The exciton-plasmon coupling is controlled by the local photonic density of states (LDOS) of the CN array. From calculations of the photonic LDOS[1,4], one can estimate the energy dispersion relation due to the exciton-plasmon coupling in the CN array. We show that due to the array periodicity, this energy dispersion relation exhibits a band structure. Thus, our predicted result is the formation of a photonic band structure in periodic densely packed nanotube arrays, which may give rise to tunable optoelectronic devices and other applications. D.D. is supported by the US NSF (ECCS-1306871). I.V.B acknowledges support from US DOE (DE-SC0007117).

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[4] I.V. Bondarev and Ph. Lambin, ``Trends in Nanotubes Research,`` Ed. D.A. Martin, Nova Science Publishers (2005).

H16: Gray-arsenic as a promising candidate for thermoelectric applications

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Thermoelectric devices that utilize the Seebeck effect convert heat flow into electrical energy. The conversion efficiency of such a device is determined by its figure of merit or ZT value, which is proportional to Seebeck coefficient and the ratio of its electrical conductivity to its thermal counterpart. To improve the ZT value, we consider various factors such as band gap size that determines Seebeck coefficient, mobility, material dimension and so on. Under these considerations, we choose two-dimensional gray arsenic, which exhibits a band gap of $\sim 1.5\text{eV}$ and high hole mobility. Such superior electronic and transport properties suggest that gray arsenic may have a potential for thermoelectric applications. We use density functional theory to investigate its thermoelectric property by evaluating its electrical conductivity, Seebeck coefficient, and thermal conductivity contributed from both electrons and lattice vibrations based on Boltzmann transport theory. Furthermore we exactly estimate relaxation time or electron-phonon scattering rate, which is an essential value for various transport coefficients, by performing a first principle calculation of electron-phonon interaction using density functional perturbation theory and wannier interpolation. We discuss the effect of the relaxation time on the thermoelectric property of gray arsenic.

H17: Kohn anomaly and quantum interference of one- and two-phonon Raman spectra in graphene

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The existence of the gapless linear energy bands (Dirac cones) in graphene modifies the phonon Raman spectra. The Kohn anomaly (KA) effect is one example that phonon energy is renormalized by excitation of electron-hole pairs in the Dirac cones, giving rise to systematic phonon frequency shift and spectral broadening upon changing the Fermi energy of graphene by doping. Although KA effect in one-phonon Raman spectra (KA1) of graphene has been studied both theoretically and experimentally, KA effect in two-phonon Raman spectra (KA2) remains intriguing topics. Several experimental results report that both phonon frequency shift and spectral broadening as a function of the Fermi energy of KA2 behave oppositely when compared to KA1. Meanwhile other experiments show asymmetric KA2 at negative and at positive Fermi energies. In this work, we calculate Fermi energy dependence of one- and two-phonon Raman spectra within tight binding method. KA effect is included in the correction of phonon energy by the second-order perturbation of electron-phonon interaction. We find that the opposite behavior of KA2 compared to that of KA1 is due to competition of interband and intraband transitions of electron-hole near the Dirac cone. Interband (intraband) transition is dominant in KA1 (KA2) due to zero (non-zero) phonon momentum takes place in the Raman process. We also find that the asymmetric KA2 comes from the asymmetry of electron and hole band structures. In one-phonon Raman intensity calculation, we confirm that the phase of Raman amplitude for incident resonant condition is opposite to that of scattered resonant one. This means if we can set the Fermi energy close enough to half of laser excitation energy, we can inhibit electron-hole transition near the scattered resonance and therefore Raman intensity changes by tuning the Fermi energy due to the quantum interference effect. This technique uncover the observation of Raman phase that could not be done before.

H18: Magnetically induced currents in empty and endohedral fullerenes

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The aromatic character of fullerenes can be discussed either as a local phenomenon where locally aromatic patterns are identified, or as a global phenomenon where the aromatic character of spherical objects is suggested to be predicted by the $2(N+1)^2$ rule for the number of delocalized π electrons. For example, C_{60}^{10+} with 50 π electrons [$=2(4+1)^2$] falls into the latter category and sustains a strong ring current that is delocalized over the fullerene surface. [1] Local aromatic stabilization could on the other hand be expected in some endohedral metallofullerenes, where electrons are transferred from the confined metal cluster to the fullerene. Localization of the transferred electrons often stabilize the complex and this stabilization could in part be due to formation of locally aromatic multi-ring moieties fulfilling the Hückel $4N+2$ rule on the fullerene. This has been suggested for the $Sc_3N@C_{68/78}$ fullerenes. [2] By the ring-current criterion, aromatic compounds such as benzene, sustain net

diatropic ring currents. In antiaromatic molecules, the net current is paratropic. If the dia- and paratropic ring-current components are equal and cancel, then the net current is zero and the molecule is nonaromatic. The ring-current delocalization patterns in fullerene molecules and the ring-current strengths at specific bonds can be determined using the Gauge-Including Magnetically Induced Currents (GIMIC)-method. In this work, the GIMIC method is applied at selected empty and endohedral fullerenes in order to investigate their possible local and global aromaticity.

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H19: One-dimensional transport in hybrid metal-semiconductor nanotube systems

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Encapsulating metallic wires of just one atom thick into a single wall carbon nanotube (CN), metallic or semiconducting, is known to drastically alter the transport properties of the compound hybrid system. For example, metallic single wall CNs encapsulating Eu metal atomic wires (AWs) exhibit extra conduction channels to supplement an overall "Tomonaga-Luttinger liquid"-like transport behavior[1]. Also interesting are hybrid metal-semiconductor nanotube systems composed of metal AWs encapsulated into semiconducting CNs. Electron transport in these hybrid structures is expected to be contributed by the AW alone at low bias voltages as there are no conduction channels available in the fundamental forbidden gap of semiconducting CNs. One might also anticipate CN mediated near-fields to affect the AW transport in these hybrid structures. Here, we study the inter-play between the intrinsic 1D conductance of metallic AWs and CN mediated near-field effects for semiconducting single wall CNs that encapsulate AWs of finite length[2]. The theory we develop predicts Fano resonances in the electron transport through the system, whereby the interaction of electrons on the wire with the CN plasmon generated near-fields blocks some of the AW transmission channels to open up a new coherent plasmon-mediated channel in the CN forbidden gap outside the AW transmission band. This makes the entire hybrid system transparent in the energy domain where neither wire, nor nanotube is individually transparent. Our work offers conceptually new ways to control and optimize charge transfer in hybrid nanodevices built on metal-semiconductor nanotube systems.

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[2] M.F.Gelin and I.V.Bondarev, *Phys. Rev. B* 93, 115422 (2016).

H20: Performance projections for ballistic carbon nanotube FinFET in circuit-level

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A novel three-dimensional device structure for carbon nanotube (CNT) fin field-effect transistor (FinFET) based on high density aligned CNT array is proposed here. Using a compact model in ballistic transport region, we simulated and evaluated the potential of CNT FinFET with Si FinFET as a benchmark at 22 nm technology node in circuit level using three performance metrics including propagation delay, total power dissipation and energy-delay product (EDP), along with their dependence on CNT spacing, supply and threshold voltages. It is shown that CNT FinFET presents more than 2 times larger current density than conventional planar gate FET (PGFET), indicating the potential to provide about 2/3 larger room for shrinking the area (or width of channel) of transistors while maintaining the same driving ability. What's more, compared with Si FinFET, the CNT FinFET presents obvious advantage in speed and EDP arising from its almost much larger current density, but which also results in higher total power dissipation especially at a low threshold voltage ($V_{th}=1/3V_{dd}$). However, a suitable improvement of V_{th} can effectively contribute to significant suppression of leakage current and power dissipation, and then an obvious optimization is obtained on EDP with an acceptable sacrifice in speed. A multi-threshold voltage scheme is then systematically simulated and suggested to construct high-performance and low-power integrated circuits (ICs). In particular, CNT FinFETs with optimized threshold voltage can provide about 50 times EDP advantage over Si FinFETs under low supply voltage ($V_{dd}=0.4$ V), suggesting huge potential of CNT FinFETs based ICs.

H21: Selective coherent phonon generations in single wall carbon nanotubes

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Ultrashort laser pulses given to a single wall carbon nanotube (SWNT) sample with duration less than a phonon period in the SWNT may generate lattice oscillations coherently, which is usually called as the coherent phonons [1]. Recently, by using sub-10-fs laser pulses, more than 10 coherent phonon modes with frequency around 100-3000 cm^{-1} could be observed in an enriched SWNT sample [2]. This finding opened up possibility to utilize particular coherent phonon modes of the SWNT as a nanoresonator with a wide frequency range in the THz regime. However, in order to take advantage of each coherent phonon mode in the real applications [3], we have to select a single coherent phonon mode with a well-defined frequency among many

phonon modes that have been excited. In this work, we theoretically investigate the ultrafast pulse-train technique to enhance a coherent phonon mode while suppressing the other phonon modes in SWNTs. In particular, we focus on the selectivity of the radial breathing mode (RBM) and the G band for a given SWNT. By adjusting the laser pulse width and pulse train repetition rate, we find that if the repetition period matches with integer multiple of the RBM phonon period, the RBM coherent phonon amplitude could be enhanced and the other modes could be suppressed. As for the G band, when we apply a repetition rate of half-integer multiple of the RBM period, the RBM could be suppressed because of destructive interference, while the G band still survives. By understanding the selectivity of each phonon mode, we expect that it could be possible to develop SWNT phononic devices in the near future.

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H22: Self-organization of doxorubicin and selected dyes molecules in inner cavity of carbon nanotubes functionalized by folic acid. A molecular dynamics study

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Carbon nanotubes (CNT) are widely studied as components of drug delivery systems because they provide an exceptionally high drug loading capacity and possibility to bind more than one functional group due to their large surface area. Drug molecules can be accommodated either to the external surface of the nanotubes or to their inner cavity. Drugs that are encapsulated within the nanotube interior are isolated from environment and protected against premature activation, degradation and reaction with healthy cells. In such a case the encapsulated drug molecules need to be locked by some caps, which can be removed by some triggering factor. We have recently found that sequential absorption of doxorubicin and some dyes molecules in the inner space of CNT can form pH sensitive drug carrier being able to release drug molecules at acidic conditions. The dye serves as a blocker of doxorubicin molecules encapsulated in the inner cavity of the nanotube at the physiological pH (pH 7.4) and it escapes at acidic pH. The organization of the fluid inside nanotubes obviously depends on the choice of dye molecule and presence of functional moieties on the external walls of the nanotube. In this study, we particularly focused on the effects coming from creation of folic acid layer on the CNT sidewall. We found that the presence of folic acid fragments significantly affects the organization of doxorubicin and dye mixture in physiological fluid. We found stable state at neutral pH and observed spontaneous release of dye and doxorubicin at acidic pH. That phenomenon can be utilized in development of novel smart drug delivery systems.

H23: Shaping electronic image states around segmented nanotubes

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Electronic image states hovering around carbon tubes were predicted and later observed in the early 00's. In this work, it is shown how to engineer multiple interacting electronic image states by manipulating the tubes of specific geometries. Because these tubular image states are highly polarizable and long-lived, they are susceptible to control by external fields. Applications for quantum logic and Rashba-type spin-orbit coupling will be discussed [1].

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H24: Stress as decisive parameter in the selective hydrogen etching of SWNTs

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While selective etching of CNTs has already been demonstrated, the underlying reasons remain elusive as yet [1]. Particularly, the precise etching nature of the H₂ plasma in the initial stage is still not fully understood [2]. We here present computational and experimental evidence to understand the onset of the selective SWNT etching in H₂ plasma. Employing hybrid MD/MC simulations, we demonstrate that during the adsorption of H atoms and their consecutive coalescence, adsorbed ortho hydrogen pairs on SWNTs induce higher shear stresses than axial stresses, leading to the elongation and eventually breaking of HC-CH bonds as a function of their alignment with the tube axis (γ -angle). We found that the ortho H pairs more perpendicular to the tube axis ($\gamma \rightarrow 0^\circ$) are responsible for C-C bond breaking in nanotubes. Also, typical UV-vis-NIR absorption spectra of HiPco experiments show that the etching probability of (semiconducting) CNT decreases with an increase of γ , which is consistent with our calculation results. Our study indicates that the chirality dependent γ -angle, in addition to the nanotube curvature and its electronic structure, is one of the key parameters in the selective etching of CNTs.

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[2] U. Khalilov, A. Bogaerts, E.C. Neyts, *Atomic scale simulation of carbon nanotube nucleation from hydrocarbon precursors*, Nat. Commun., **6**, 10306, 2015.

H25: SWNT growth modes and selectivity studied by computer simulation

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We use computer simulation techniques [1, 2] to address important issues relevant to Single Wall Carbon Nanotube (SWCNT) growth by Catalytic Chemical Vapor Deposition. We evidence different SWCNT growth modes so-called “tangential” and

“perpendicular”, as shown in Fig. 1. Such behaviors can be generalized for various catalyst nanoparticle (NP) / tube diameter ratios. We emphasize the key role played by carbon solubility in the NP during SWNT synthesis.

A detailed analysis of the energetics of SWCNTs in contact with NPs, shows that their diameter can be controlled by the carbon concentration in the catalyst during growth. In the case of Nickel and similar catalysts, tangential and perpendicular growth modes ultimately result from the carbon concentration dependence of the wetting properties of the catalyst with respect to the SWCNT wall. These behaviors are supported by recent experimental results [3, 4]. Finally we discuss our current understanding of the SWNT growth mechanisms and its chiral dependence.

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[4] M. He *et al.*, submitted 2016

H26: Theory of UV to THz light conversion using graphene nano-ribbons

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In this presentation, we propose application of graphene nano-ribbons, which can be formed by bottom-up growth technique [1], to modulate intensity of UV optical field with THz frequency. We have performed the real-time propagation TDDFT simulation of electron of graphene nano-ribbon with presence of optical field, and monitored the induced field by electron motion in the nano-ribbon. We then observed significant field enhancement when the frequency of incident optical field is in UV region and the enhancement has a period of 100 fs (10 THz frequency) [2]. In this presentation, we discuss the mechanisms of such large field enhancement as well as THz modulation, and propose application of graphene nano-ribbons for THz radiation. This work was supported by Science of Atomic Layers (SATL), Grant-in-Aid for Scientific Research for Innovative Areas by MEXT, Japan

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[2] H. Zhang, Y. Miyamoto, X. Cheng, A. Rubio, Nanoscale **7**, 19012-19017 (2015).

H27: Thermodynamic screening of bimetallic catalysts for chirality controlled growth of carbon nanotubes

Vets, Charlotte (University of Antwerp, Department of Chemistry, Research group Plasmant, Wilrijk, BEL); Neyts, Erik (University of Antwerp, Department of Chemistry, Research group Plasmant, Wilrijk, BEL)

Chirality controlled growth of CNTs remains a topic of major importance [1]. Bimetallic catalysts provide a possible means to achieve better chirality control [2,3]. In this work, we investigate one of the factors potentially controlling chirality during CNT growth: the adsorption energy of a CNT on a bimetallic catalyst. We use Density

Functional Theory (DFT) calculations in order to first investigate the stability of several catalyst nanoparticles (NPs), in terms of their cohesive energy and formation enthalpy. Six NP alloys are simulated in various compositions and atom distributions, both without and with interstitial carbons (to mimic the dissolution of carbon in the system [4,5]). Subsequently, we use Molecular Dynamics (MD) simulations to study the melting behaviour of a selection of stable NP alloys [6], as it has been shown that chirality control is more readily achieved at lower temperatures, in which case the NP is more likely to remain in the solid state [7]. Finally, we use DFT to calculate the adsorption energies of hydrogen-passivated CNTs with various chiralities on the selected stable NPs. This thermodynamic screening can provide insights in how to steer the preference for certain chiralities.

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H28: Transverse Electric Surface Wave in Silicene

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The gapless linear electronic dispersion of graphene gives unusual optical conductivity, in which the imaginary part of optical conductivity can be negative at certain range of frequency as opposed to always positive Drude conductivity in conventional 2D electron gas [1]. It was predicted a decade ago that such an unusual conductivity behavior has allowed graphene to support transverse electric surface wave (TESW), which requires negative imaginary part of σ [1]. Different to transverse magnetic surface wave (TMSW), or well-known as surface plasmon [2,3], TESW is magnetic dipole waves [4]. Compared to TMSW, TESW can propagate farther, due to low propagation loss [5]. Recently, the existence of TESW in graphene has also been proved experimentally [4]. However, the frequency range of TESW in graphene is very narrow, at around 1.667 to twice Fermi energy [1,4] and the wave is not really confined to the surface [4,5]. In this work, we theoretically predict that another 2D material with slightly buckled honeycomb lattices, such as silicene, may also support TESW. The advantage is that we have a wider frequency range, which is electrically tune-able by external electric fields. For example, TESW frequency range can be within 0.85 to twice Fermi energy. Better TESW confinement may also be expected in silicene. We expect that such a feature is general for all 2D materials having slightly buckled honeycomb lattices.

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H29: Tuning of polarization of h-BN nanoribbons by the edge hydrogenation

Yamanaka, Ayaka (University of Tsukuba, Tsukuba, JPN); Okada, Susumu (University of Tsukuba, Tsukuba, JPN)

Hexagonal boron nitride (h-BN) is attracting much attention as an insulating version of graphene, owing to its unique physical properties, such as mechanically strong hexagonal covalent network, high thermal conductivity, and an insulating electronic structure with wide band gap. Because of these properties, h-BN is regarded as a potential material being applicable for the wide areas in the current and future nanotechnologies. For practical applications of h-BN, it is mandatory to understand their fundamental properties. In this work, we study the electronic structure of h-BN nanoflakes with various edge structures to give a theoretical insight into the physical properties of h-BN. All calculations are performed by using the density functional theory (DFT) with the generalized gradient approximation. The effective screening medium (ESM) method is applied to avoid the unphysical dipole interactions with the periodic images. Our calculations showed that the potential difference between the right and left edges of hydrogenated nanoribbons is opposite to that of nanoribbons with clean edges. The potential difference also depends on the edge shapes of h-BN nanoribbons. Nanoribbons do not have potential difference in both hydrogenated and clean edges with armchair shape. With increasing zigzag portion, the potential difference monotonically increases for the hydrogenated nanoribbons. On the other hand, potential difference possesses the almost constant values irrespective to the edge shapes for the clean edges. The facts indicate that the edge shapes and termination can control the polarization of h-BN nanoribbon.

H30: Understanding the onset of CNT growth by hybrid MD/MC simulations

Khalilov, Umedjon (University of Antwerp, Antwerpen, BEL); Neyts, Erik (University of Antwerp, Antwerpen, BEL)

In spite of recent advances, the onset of the carbon cap and nanotube nucleation process is still not fully understood. We here study the atomistic mechanisms of cap nucleation and the role of carbon precursors, including pure, hydrogen and oxygen-based carbon species in the initial stage of the growth process. All simulations were carried out by means of hybrid MD/MC simulations on either Al-bound or Si-bound Ni clusters in the temperature range 1000-2000 K. We distinguish and analyse three consecutive stages in the onset of CNT growth: incubation, cap formation and continued CNT growth [1]. We found that C atoms may either diffuse into the cluster after full dehydrogenation, or diffuse over the surface in the case of partial dehydrogenation during the growth from hydrocarbon species. In either case, they are found to eventually incorporate into the carbon network. On the other hand, in the case of oxygen-based carbon precursors, after their adsorption and dissociation, the O atoms mostly desorb as H₂O molecule due to finding two surface hydrogen atoms on the cluster. Also, in both precursor cases, the appearance of unstable C

structures in the incubation stage of in-situ TEM observations [2] and the onset of MWNT nucleation through the formation of a multi-layer graphene structure [3] are carefully discussed [1,4]. The obtained results are in good agreement with available experimental and quantum-mechanical results, and provide a basic understanding of the incubation and nucleation stages of CNT growth at the atomic level.

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[4] U. Khalilov, A. Bogaerts, E.C. Neyts, *Nanoscale*, **6**, 9206, 2014.

H31: Unloading of drugs molecules from carbon nanotubes inner cavities by pH change insights from molecular dynamics simulations

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An important feature of carbon nanotubes is the presence of a hollow and open internal space. That space can collect other molecules, particularly small molecule drugs, so those molecules can be perfectly isolated from the environment. It needs, however, creation of removable caps, which locks/unlocks those guest molecules in response to some triggering factor, e.g. the pH change from neutral to acidic one occurring in tumor tissue. [1] In this study, we analyzed two architectures which can realize pH controlled corking and uncorking of carbon nanotubes. The first architecture uses small gold nanoparticles linked with the nanotube by hydrazone bond containing fragments. [2] The second one utilizes co-absorption of some dyes molecules and drugs in the inner cavity of carbon nanotube. In both cases we observed stable capped states of the nanotube at neutral pH while at acidic pH the caps (either gold nanoparticles or clusters of dyes molecules) remove spontaneously provided that some specific conditions are satisfied. Our results show that by applying theoretical analysis of the above mentioned processes we can understand their mechanisms on the molecular level, find the most critical steps and draw conclusions concerning the applicability of the discussed architectures as pH controlled drug delivery systems.

Acknowledgement: This work was supported by National Science Centre (NCN) grant DEC-2012/07/E/ST4/00763.

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H32: Young's modulus Estimation of fullerene nanostructure by using molecular mechanics and finite element method

Nayebi, Ali (Shiraz University, Shiraz, IRN); Ghavanloo, Esmael (Shiraz University, Shiraz, IRN)

In this paper, a three-dimensional finite element model is proposed for estimating Young's modulus of fullerene nanostructures. The model is based on the assumption that the fullerenes, when subjected to loading, behave like space-frame structures. The bonds between carbon atoms are considered as connecting load-carrying members like beams under axial, bending and torsion loadings, while the carbon atoms as joints of the members. To create the finite element models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional elastic beam elements. The elastic modulus of beam elements is determined by using a linkage between molecular mechanics and continuum mechanics. In order to evaluate the Young's modulus, the spherical shell theory is also utilized. Compression loading on the fullerene is considered and the load – displacement variation is obtained. The effect of diameter on the elastic modulus of fullerenes nanostructures has been studied and it is observed that by increasing the radius of fullerenes, their elastic modulus decreases. After studying the properties of perfect fullerenes, the Young's modulus of different defective fullerenes is also determined.

POSTER SESSION I: Graphene & van der Waals Heterostructures

I1: Analysis of radiation sensitive defects, structures and molecules on graphene

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With today's aberration corrected machines, atomically resolved (scanning) transmission electron microscopy (TEM/STEM) has become a standard characterization technique for nanoscaled materials, especially in the evolving field of 2D-materials. However, a big limitation is beam damage because of the high required dose of energetic electrons. While reducing the acceleration voltage to 80 kV or below can prevent beam damage in pristine graphene, defects, functional groups or molecules on the surface are still strongly affected by energetic electrons. Our recently published algorithm [1, 2] makes it possible to reconstruct defects or single molecules on graphene from simulated STEM and TEM low-dose data. In this approach, the electron dose is distributed over many copies of the same structure which makes it possible to directly image the atomic configuration of highly beam-sensitive materials in the TEM. Depending on the dose, areas up to a few square micrometer have to be imaged with atomic resolution which corresponds to up to several thousand single single images. Acquiring such amounts of data efficiently is only possible via automated methods. We present such an approach implemented on our Nion UltraSTEM 100.

[1] Ultramicroscopy, Vol. 145, pp. 13-21, 2014

[2] Ultramicroscopy, submitted, 2016

I2: Fabrication of Schottky type solar cell with few-layer transition metal dichalcogenide

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Atomic scale 2D sheets attract intense attention due to their superior electrical, mechanical, and optical features. Layered transition metal dichalcogenide (TMD) is known as a true 2D material with excellent semiconducting properties [1]. TMD is one of the most attractive materials for future high performance transparent and flexible solar cells due to their atomically thin structure, band gap in visible light range, and high optical transparency. Although the solar cell of TMD has been widely investigated by many groups, those are based on the pn-junction or hetero-junction type solar cell. Since complicated structures are required to form pn junction or hetero-junction structures in TMD such as dual gate electrodes and position selective layer-by-layer stacking, the device size of these solar cell with TMD is limited within

very small region (few μm). The schottky type solar cell is known as another type of solar cell and it is possible to scale up the device up to the practical size because of the simple device structures. However, the detailed study of schottky type solar cell with mono or few-layer TMD has not been reported. Because the schottky barrier is formed at the contact region between electrode and TMD, it is important to select appropriate electrode pairs for left and right electrodes. In this study, we have investigated the combination of left and right electrodes and the distance of each electrode to obtain the better performance. Through the adjustment of these factors we have succeeded in the fabrication of the high performance schottky type solar cells with few-layer WSe₂.

[1] T. Kato and T. Kaneko, ACS Nano 8, 12777 (2014).

I3: Gate-Tunable Landau level Filling and Spectroscopy in Coupled Massive and Massless Electron Systems

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We will present the results of transport studies on coupled massive and massless electron systems, realized using twisted monolayer graphene/natural bilayer graphene stacks encapsulated in BN. We incorporate the layers in a dual-gated transistor geometry enabling independently tuning their charge density and the perpendicular electric field. In a perpendicular magnetic field, we observe a distinct pattern of gate-tunable Landau level crossings. Screening and interlayer electron-electron interactions yield a nonlinear monolayer gate capacitance. Data analysis enables determination of the monolayer's Fermi velocity and the bilayer's effective mass. The mass obtained is larger than that expected for isolated bilayers, suggesting that the interlayer interactions renormalize the band structure.

I4: Growth of integrated graphene films with high crystallinity

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In the field of high-speed transistors, integrated graphene films consisted of single-layer graphene channel with high carrier mobility and multi-layer graphene electrodes with good conductivity would be appreciate. In this study, we introduced a growth technique of integrated graphene films with high crystallinity and uniformity. The catalytic substrate was consisted of Ni and Cu films with TiN film as a diffusion barrier for two catalytic metals and aggregation suppression layer for Ni thin film, resulting in a growth of multi-layer graphene electrode with uniform thickness. Observations on growth process could give a comprehension of the growth mechanism for integrated graphene films. The fabricated devices with integrated graphene films showed the advanced performance.

I5: High-resolution electron microscopy of 2D materials growth and 2D/non-2D integration

Bayer, Bernhard (Physik Nanostrukturierter Materialien, Wien, AUT); Caneva, Sabina (University of Cambridge, Cambridge, GBR); Aria, Adrianus (University of Cambridge, Cambridge, GBR); Kaindl, Reinhard (Joanneum Research, Niklasdorf, AUT); Kratzer, Markus (University of Leoben, Leoben, AUT); Waldhauser, Wolfgang (Joanneum Research, Niklasdorf, AUT); Teichert, Christian (University of Leoben, Leoben, AUT); Hofmann, Stephan (University of Cambridge, Cambridge, GBR); Meyer, Jannik (University of Vienna, Vienna, AUT)

The translation of two-dimensional (2D) nanomaterials such as graphene, hexagonal Boron-Nitride (h-BN) or Molybdenum Disulfide (MoS_2) into real world applications critically hinges on industrially scalable growth as well as seamless and scalable integration of the novel 2D materials with a wide range of other established functional non-2D (nano-)materials such as metals, metal-oxides or organic semiconductors. The underlying growth mechanism and resulting structural, chemical and electronic interfacing effects remain however largely elusive, in particular on the atomically resolved level. This precludes rational 2D growth and 2D/non-2D integration process design. Here, we show recent examples of how atomically-resolved scanning transmission electron microscopy (STEM), combined with bright-field and dark-field transmission electron microscopy (TEM) techniques, can provide the critically required physical and mechanistic insights: In a first example, we elucidate non-equilibrium layer stacking and a controlled grain boundary structure in h-BN layers grown by scalable chemical vapour deposition (CVD) [Nano Lett., 16, 1250 (2016)]. Further, we examine atomic layer deposition (ALD) of the important high-k dielectric HfO_2 on CVD graphene and identify HfO_2 nucleation modes on graphene. As an alternative to CVD, we also examine physical vapour deposited (PVD) MoS_2 layers on CVD graphene and evidence electron-beam induced MoS_2 crystallisation and the possibility of epitaxial MoS_2 -graphene integration. Finally, we discuss the use of (S)TEM to study the competing effects of epitaxy and preferential nucleation in the growth of organic semiconductor molecule films on CVD graphene [Appl. Phys. Lett., 106, 103101 (2015)].

I6: Semiconducting Electron Transport in Graphene Induced by Periodic Uniaxial Strain

Kanda, Akinobu (University of Tsukuba, Tsukuba, JPN); Hiraide, Rineka (University of Tsukuba, Tsukuba, JPN); Sonoda, Hiroki (University of Tsukuba, Tsukuba, JPN); Higuchi, Shoma (University of Tsukuba, Tsukuba, JPN); Tomori, Hikari (PRESTO-JST and University of Tsukuba, Tsukuba, JPN)

Lattice strain in graphene produces pseudo- vector and scalar potentials, leading to band modulation and formation of Landau-level-like band gap.[1] Such a band gap has so far been observed in local probe measurements using scanning tunneling spectroscopes or nano-probers[2], in which strain was induced by placing graphene on top of a nanostructured substrate. On the other hand, any strain-induced band gap has never been seen in field effect devices that have source/drain and gate electrodes.

It is speculated that the wet process in the device fabrication relaxes the strain. In this study, we develop a method of fabricating field effect devices of graphene with designed spatial variation of strain. In a graphene field effect device with periodic uniaxial strain, transport measurement confirms the formation of strain-induced band gap. In our novel sample fabrication method, a graphene film is placed on top of a corrugated surface of the substrate but the introduction of strain to graphene is prevented during the electrode formation process. This is done by sticking the graphene film to a thick supporting layer. In the back gate voltage (V_g) dependence of the conductance in the periodically strained graphene, the minimum conductivity exhibits thermal activation behavior at high temperatures (> 50 K). From the Arrhenius plot, the band gap is estimated to be ~ 2.4 meV. Besides, the current-voltage characteristics become nonlinear around the origin. The high resistance region extends in a region of ± 2 meV at $V_g \sim 40$ V, which agrees with the band gap estimated from the temperature dependence. These observations confirm the formation of the band gap in our strained graphene. We expect that optimization of the device structure extends the gap and improves device performance.

[1] F. Guinea et al., Nat. Phys. 6 (2010) 30.

[2] J. K. Lee et al., Nano Lett. 13 (2013) 1394; K. K. Bai et al., Phys. Rev. Lett. 113 (2014) 086102.

I7: Study of Local Deformation of 2D-Materials by Dual-Probe AFM/STM

Hummel, Stefan (University of Vienna, Vienna, AUT); Elibol, Kenan (University of Vienna, Vienna, AUT); Bayer, Bernhard C. (University of Vienna, Vienna, AUT); Kotakoski, Jani (University of Vienna, Vienna, AUT); Meyer, Jannik C. (University of Vienna, Vienna, AUT)

Strain engineering is a very promising tool for changing the physical properties of 2D materials. In recent years, different experimental and theoretical studies have shown that graphene and other two dimensional materials (2D) (e.g. MoS₂) are very sensitive to strain regarding charge transport, electrical and phononic band structure, etc. Up to now, most experimental methods for the investigation of strain induced effects on 2D materials are based on either employing micro electromechanical (MEMS) devices or applying uniaxial strain by using a flexible substrate. In these experiments, one is either limited in sample size due to the MEMS structure or has to account for the underlying substrate. In this work, I will show recent results of a novel type of strain measurement based on a Dual-Probe atomic force-(AFM)/scanning tunneling- (STM) microscope setup, where the two probes approach a suspended membrane from opposite sides. With this setup, we can explore local deformations of 2D materials caused by an approaching STM tip, while performing AFM measurements on the same site. Using a conductive AFM tip, I will also present new possibilities of electrical two-probe measurements, where the lateral distance of the two probes is not restricted by any manufacturing limitations and hence, can in principle be performed on the same atom.

I8: Studying deformed 2D materials via hybrid AFM/Raman and dual-probe STM/AFM

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Using hybrid AFM/Raman spectroscopy and dual-probe STM/AFM, we demonstrate how the local AFM/STM tip used as a nanoindentation probe on the free-standing material influences the mechanical and electrical properties of the two-dimensional materials. Due to the fact that highly localized deformation leads to strained atomic structures, a variety of physical and chemical properties of the two-dimensional materials including electrical, thermal and mechanical properties is altered. Experiments in our study were carried out on the free-standing 2D materials graphene and Molybdenum disulfide (MoS₂). In hyperspectral Raman mapping experiments, we induce a local strain on two-dimensional materials (in this experiment, we use few layer graphene “FLG” as a model system) by an AFM probe and visualize the strain distribution under and around the AFM tip by mapping the strain-dependent frequency shifts of the few layer graphene’s G and 2D Raman bands. In a separate experiment, we induce and measure deformations via a uniu dual-probe STM/AFM where a free-standing membrane can be probed from both sides. In this case, the mechanical and electrical cross-talks across the thin membrane provide insights into both the tip-sample interaction as well as into electrical and mechanical properties of the membrane.

I9: Atomic resolution imaging of structural defects in Graphene and MoS₂

Ludacka, Ursula (University of Vienna, Wien, AUT); Hummel, Stefan (Herr, Wien, AUT)

We present a scanning transmission electron microscopy study of defects in graphene and nanopores in MoS₂, which epitomize the family of two-dimensional materials. To transform a pristine, hexagonal graphene membrane into a disordered 2D carbon structure containing pentagons, hexagons, heptagons and octagons, we used electron beam irradiation. The rate of amorphization due to increasing defect density was monitored via changes in the observed diffraction pattern. To hinder the destructive effects of chemical etching during the process, these experiments were carried out at 150 °C. By contrast, MoS₂ monolayers were irradiated with 7000 Xe₃₀ ions/μm² and 500 Xe₄₀ ions/μm². The atomic structure of the created defects was later imaged with a Nion UltraSTEM 100, operated at 60 kV. In addition to static atomic resolution imaging of vacancies and impurity atoms, dynamical behavior, such as their movement through the lattice as well as bond rotations were observed. Detailed analysis of both of the structural defects in graphene and the pore size distribution in MoS₂ will be presented.

I10: Air-stable carrier doping into nano-carbon materials by extraordinary molecular Lewis acid

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Graphene and carbon nanotube (CNT) thin films are expected as one of the promising materials for next-generation transparent electrodes due to their high transparency, electrical transport properties, and high flexibility. However, the sheet resistance of these nano-carbon materials is higher than that of indium tin oxide films, which is used as transparent electrodes commonly. Therefore, it is important to decrease their resistance by a chemical doping method. In addition, since chemically-doped nano-carbon films are not air-stable in previous researches, air-stable carrier dopants are strongly required for practical application [1, 2]. More concretely, in our study, we focus on the combination of the extraordinary molecular Lewis acid, diarylborinium ion (Mes_2B^+ ; Mes (mesityl) = 2, 4, 6-trimethylphenyl) and thermally-stable counter anion, tetrakis (pentafluorophenyl) borate ($[(\text{C}_6\text{F}_5)_4\text{B}]^-$) as novel air-stable dopants [3]. We prepared few-layer graphene and CNT thin films, and immersed them into the saturated o-dichlorobenzene solution of the dopants. After that, we conducted four-probe resistance, the Hall effect, thermopower and transmittance measurements for non-doped and doped films. As the results, we obtained high hole carrier density ($> 10^{14} \text{ cm}^{-2}$), strong sheet resistance reduction ($> 60\%$) and one-month air stability without significant decrease of transmittance. Importantly, the air-stability of our dopants was better than that of previous researches, such as HNO_3 , and others [1, 2]. In summary, we succeeded in air-stable hole doping into graphene and CNT thin films by the extraordinary dopants ($\text{Mes}_2\text{B}^+[(\text{C}_6\text{F}_5)_4\text{B}]^-$), which promotes the future application.

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I11: Anomalous stacking structures in graphene oxide treated at ultrahigh temperature in ethanol environment

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The restoration of graphitic structures from defective graphene oxide (GO) was examined in a ethanol environment at ultrahigh temperatures [1]. Dry GO flakes composed of aggregated single-layer GO were used as the samples. The GO processed in ethanol at 1800 °C exhibits much better features of D- and G-bands in Raman

spectra and its crystallinity is comparable to that of CVD-grown graphene. The stacking order of the processed GO was analyzed by 2D-band shape in Raman spectra and X-ray diffractometry (XRD). The 2D-band analysis for the GO processed under inert (N₂ or Ar) environment at 1800 °C indicates that the volume ratio of Bernal stacking in the processed GO was ~70 %. In contrast, GO processed in ethanol environment gave rise to the ratio of ~30 %. This result means that turbostratic structures are preferentially formed by the ultrahigh-temperature process in ethanol, suggesting the effect of ethanol for suppressing the GO graphitization at ultrahigh temperatures. Crystalline size in c-axis direction (L_c) and interlayer distance of processed GO were analyzed by the width and peak position of (002) signals in XRD pattern. Evaluated L_c and interlayer distance of the processed GO indicate the almost same values for ethanol and inert environments. This result of XRD is quite contrary to that of the 2D-band analysis in Raman spectra. This inconsistency between the analyzed results may arise from the difference of probing depth for the both analysis methods: Raman spectroscopy detects only the topmost surface (~10 nm) of graphene, and XRD observes almost all samples. Consequently, these results indicate that highly crystalline graphene with turbostratic structure was formed near the surface of processed GO, and GO thin films (several nm thick) processed at ultrahigh temperatures in ethanol should be promising for applications of turbostratic graphene, such as quasi single-layer electronics in future studies.

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I12: Ballistic transport in graphene antidot lattices

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We observed commensurability magnetoresistance arising from ballistic electron transport in the triangular antidot lattice of high-mobility graphene that was made on h-BN. For the monolayer and bilayer graphene antidot devices with carrier mobility of about 3x10⁴ cm²/Vs and mean free path of about 400-600 nm, we observed bipolar magnetoresistance peaks that originates from commensurability of a cyclotron orbit with antidot lattice. Detailed study of the magnetoresistance peak as a function of carrier density revealed that the commensurability occurred when cyclotron diameter matches lattice constant, i.e, 2R_c=a, where R_c is the cyclotron radius and a is a lattice constant. [1] Shapes of the magnetoresistance traces were approximately reproduced by numerically calculating conductivity components using the semiclassical Kubo type formula for chaotic orbits. The peaks appeared when the carrier mean free path was approximately larger than the lattice constant of the antidot, which quantitatively agreed with our experiment. We observed another commensurability effect showing suppression of Shubnikov-de Haas (S-dH) effect in low field regime. This arose from intervention of cyclotron orbit by scattering with antidots. At a magnetic field satisfying a condition 2R_c=a-d, where d is diameter of an

antidot, phase volume of the states for complete cyclotron orbit, begins to increase steadily, thereby clear S-dH effect appears. These results clearly demonstrated ballistic transport of Dirac electron systems.

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I13: BiOpClq/BiOxIy/GO composites: Synthesis, characterization, and photocatalytic activity

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In recent years, toxic organic dyes and their effluents become one of the main sources of water pollution because of the greater demands for industry. Semiconductor photocatalysis driven by visible light has sparked enormous research interest because it provides a promising pathway for solving energy supply and environmental pollution problems. Graphene-oxide (GO) has attracted great attention because of its unique properties similar to graphene, such as its special surface with hydroxyl and carboxyl groups introduced, which were fabricated for the synthesis of GO-containing composites. Particularly, great efforts have been devoted to the preparation of semiconductor/GO composites, aiming to improve the photocatalytic efficiency. In this study, a series of BiOpClq/BiOxIy/GO were prepared using controlled hydrothermal methods. The GO powder was prepared using the improved Hummers method with additional KMnO₄. The compositions and morphologies of BiOpClq/BiOxIy/GO could be controlled by adjusting some growth parameters, including reaction pH value, temperature, time, and KCl and KI. The structures and morphologies of BiOpClq/BiOxIy/GO were characterized by XRD, HR-TEM, SEM-EDS, FT-IR, HR-XPS, DR-UV, BET, and CL. The as-prepared samples were tested for the photocatalytic degradation of Crystal Violet. The study is useful in synthesizing BiOpClq/BiOxIy/GO and degrading dye for the future applications of environmental pollution and control.

I14: Charge carrier scattering on pseudomagnetic field profiles in graphene

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Mechanical strain in graphene creates pseudomagnetic fields which can have dramatic consequences on the behavior of electrons and holes. Here we show that pseudomagnetic field fluctuations can induce significant intravalley scattering of charge carriers. These processes are detected in Raman scattering measurements via the anomalous intensity of the D' peak with respect to the D peak. Furthermore, anomalous laser energy dependence of the relative peak intensities emerges. Our theoretical model can reproduce both features. Our work confirms that it is possible to optically detect the presence of pseudomagnetic field fluctuations.

I15: Enhanced Raman Scattering of Graphene with Density and Location of Silver Nanoparticles

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Graphene-metal nanoparticle heterojunction, greatly enhance the surface-enhanced Raman scattering (SERS) by the strong light-graphene interactions, is at the center of significant research effort. In this work, we used large size Ag nanoparticles (NPs), either underneath or on top of the graphene, to enhance the Raman scattering. Herein, Raman scattering from graphene is significantly enhanced with the different density of the Ag NPs at the same location. Meanwhile, there is present of an obvious red-shift and broadening in the resonance peak of Ag NPs, which may be correlated with the strength of Raman enhancement and the coupling of the deposited Ag NPs and the graphene. In addition, graphene-Ag NPs heterojunctions can be used as SERS substrates to enhance Raman signals of the rhodamine (R6G) molecules and suppress photoluminescence (PL) signals from the Ag NPs. Based on the tunable Raman enhancement, graphene-Ag NPs may offer a promising platform for engineering SERS substrates to obtain highly-sensitive detection of trace levels of analyte molecules.

I16: Fabrication of graphene nanoribbons at step edges of SiC (0001) by selective oxygen etching of buffer layer on terraces

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Graphene nanoribbons with remarkable ballistic and high mobility transport have been formed at step edges of a SiC (0001) surface. Also, edge types (armchair or zigzag) of graphene nanoribbons can be easily controlled on a lithographically patterned SiC surface, which brings significant potential for future electric devices. However, due to a bottom-up growth process of graphene on SiC, graphene nanoribbons at step edges connect to a buffer layer on terraces^[1] which may degrade its electric properties. To improve the fabrication of graphene nanoribbons on SiC, we suggest a selective oxygen etching method to remove the buffer layers. Based on chemical stability of graphene higher than that of buffer layers, a well-controlled thermal treatment in an oxygen-argon atmosphere was found to be effective to etch only the buffer layers on SiC terraces. The etching processes were investigated by in situ scanning electric microscopy (SEM) and scanning tunneling microscopy (STM). Single layered graphene nanoribbons (width from tens to hundreds of nanometers and length over 10 μm), under which a buffer layer remained, were formed at step edges. [1] M.S. Nevius et al. *Nano Lett.* 2014, 14, 6080

I17: Geometric and optoelectronic properties of thin-layer GeSe and heterostructures

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GeSe is one of the group IV monochalcogenides that are described by analogy with black phosphorus. The monolayer and bilayer materials are direct bandgap semiconductors like monolayer MoS₂ [1,2], promising for optoelectronic applications

such as photovoltaic cells. Anisotropic spin-orbit splitting induced by inversion symmetry breaking due to binarity, unlike phosphorene, has also been reported [1,2], which may provide a new route to spintronics. For use of this material in practical applications, however, it is of the utmost importance to understand these properties in heterostructures as well as the thickness dependence. In this study, we perform first-principles calculations to elucidate the geometric and optoelectronic properties of thin-layer GeSe and its heterostructures. We found that the lattice constants and internal atomic positions of GeSe change significantly with the thickness in contrast to rigid MoS₂. Trilayer GeSe still has a nearly direct gap with anisotropic spin-orbit splitting. The split at the valence band edge is even larger than that of monolayer GeSe because the geometric change increases the Ge p orbital component around the energy. We also carried out the large-scale calculations of lattice-matched heterostructures. For heterostructures with typical layered dielectric material, hBN, we can see a direct band gap derived from GeSe, although the spin-orbit splitting is much smaller than that of isolated GeSe. A GeSe/MoS₂ heterostructure gives type II band alignment that plays important roles in optoelectronic applications. An alternate bulk heterostructure with GeS that is another group IV monochalcogenide brings a new material rather than a heterostructure; the wave functions are spread over the whole material and the band gap is even narrower than that of bulk GeS despite the wider band gap of GeS. This work was partly supported by CREST, JST.

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I18: Graphene-induced instabilities in polymer matrix

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Graphene along with other two-dimensional (2D) materials is considered as a candidate material for flexible and stretchable electronics. Graphene can also work as a reinforcing material in composites with its high mechanical stiffness. In such applications as flexible electronics or composites, interfacial interaction between graphene and the host material (often polymer matrix) is expected to play an important role. Therefore, understanding such mechanical interactions in terms of adhesion, friction, and strain at the interface is important. In this work, we investigated the interfacial mechanical interactions between graphene [grown by chemical vapor deposition (CVD)] and polymer [PMMA (Polymethyl methacrylate)] matrix. After graphene is grown by CVD, it is patterned and transferred to PMMA film, embedded in the polymer matrix. Afterwards, tensile strain on the graphene pattern is applied by swelling of the PMMA matrix (due to absorption of low molecular weight alcohol such as methanol). Stress distribution on graphene is investigated by *in situ* and *ex situ* Raman measurements. Electrical transport measurements are also performed to assess modifications of electrical properties of the device. Strong adhesion and the large difference in modulus between two materials result in the significant stress transfer and focusing at the interface, which eventually leads to the fracture of graphene and the PMMA film. A classical model

considering the role of stress transfer at the interface can explain the observed crack formations and crack patterns.

I19: H-BN/graphene heterostructures synthesized in a STEM

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The electronic band gap of graphene can be tuned by compositing graphene with materials of different band gap energies. We report the direct observation of a lateral heterostructure synthesis by epitaxial in-plane graphene growth from the step-edge of hexagonal BN (h-BN) within a scanning transmission electron microscope (STEM) chamber. The growth interface between h-BN and graphene is atomically identified mainly as N-C bonds. By using a post-growth method, graphene nanoribbon can be synthesized to connect two h-BN domains with different twisting angles, forming a lateral heterostructure ((h-BN_Gh-BN)/G), as well as isolated carbon islands with arbitrary shapes embedded in the h-BN layer. Low-loss of electron energy-loss spectroscopy (EELS) analyses of the dielectric response suggest a robust coupling effect between the graphene and h-BN layers.

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I20: Interaction of Quantum dot with MoS₂ monolayer

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Quantum dots with varying size and structures are promising materials for optoelectronic applications. While perovskites quantum dots (P-QD) have optically tunable bandgap with bright and excellent photoluminescence quantum yield; carbon dots (C-dots) have strong fluorescent, which are water soluble, chemically inert, ease to functionalize and photo-bleach resistant. Transition metal di-chalcogenides

(TMDs), represents a group of 2D layered materials that exhibit diverse properties and can be semiconductors, semi-metals, true metals or superconductors depending on their composition. Advantageous properties of both quantum confined material can be conveniently combined in a hybrid structure featuring P-QD or C-dots dispersed on a monolayer MoS₂ film. Here, we present our recent work on electrical and optical characterization of C-dots/P-QD on monolayer MoS₂ hybrid system. Electrical characterization of MoS₂/C-dot and MoS₂/P-QD device showed that the current level after laser irradiation is increased ~100 times and ~20 times in comparison to the dark. Both electrical and optical characterization showed a significant charge transfer from C-dots to MoS₂ thus increasing the n-doping in MoS₂ monolayer. The observed interesting photo induced electron transfer properties on such systems could offer exciting opportunities for light energy conversion, photovoltaic devices and related applications.

I21: Introducing Uniaxial Local Strain to Graphene Encapsulated with hBN

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Due to high mobility, graphene is a promising candidate for electronic materials. However, for successful application of graphene to switching devices, gap formation is indispensable. In this study, we explore the gap formation in graphene based on strain engineering.[1] One of the graphene's outstanding properties is that strain induces pseudo-vector and scalar potentials, which can modulate transport property of graphene. Previously, we induced uniaxial strain to graphene by inserting resist nano-rod between graphene and the substrate (SiO₂),[2] and observed the gate voltage dependence of conductivity which is asymmetric to the charge neutrality point. We attributed the asymmetry to the strain-induced pseudo scalar potential. However, zero conductivity did not seen presumably due to short electron mean free path. Here, to elongate the electron mean free path, we use graphene sandwiched between hexagonal boron nitride (hBN) films. Lattice strain is induced locally in graphene by making a hill and a valley on the inner surfaces of hBN. In the sample fabrication, we used van der Waals dry transfer and edge contact techniques.[3,4] From micro Raman spectroscopy, the maximum strain is estimated to be ~ 0.13 %.[5] In transport measurement, the conductance decreases with decreasing temperature within the whole gate voltage range. The minimum conductance exhibits thermal activation behavior at high temperatures (300 K - 40 K), indicating the existence of a transport gap. From the result, the gap is estimated to be 3.2 meV. This value is consistent with value expected from spatial variation of strain in this sample.

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I22: Investigation of carbon-nitrogen bonding state in graphene on catalytic activity

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Nitrogen-doped (N-doped) graphene promises to improve the application potential of current graphene based devices. For example, graphitic nitrogen is known to promote desired catalytic activities (oxygen reduction reaction, ORR) in graphene fuel-cell systems. While some studies have demonstrated the catalytic enhancement of N-doped graphene, they have also indicated that factors such as the location and the bonding state of the N-dopants may be determinants in graphene property design. According to previous report [1], graphitic N-dopants are better at enhancing graphene's catalytic activities— illustrating the importance of the N-dopant bonding state. However, established nitrogen-doping methods lack selectivity in dopant chemical identity and in dopant location; both are key factors in graphene property design. We have reported a post-treatment method that selectively controls the location and bonding state for synthesizing N-doped graphene [2]. Our approach uses a charge neutral nitrogen beam with tunable beam energy to insert N-dopants into graphene. We found selective synthesis of both C-N and C=N rich condition is possible by changing beam energy. In this study, we report investigation of electrochemical activity of graphitic nitrogen rich graphene. CVD grown graphene was transferred onto a rotating disk electrode. Then it was treated by neutral nitrogen beam. Electrochemical measurement was carried out in oxygen saturated 0.1 M KOH solution and N-doped graphene was used as the working electrode. Catalytic activity of N-doped graphene is found to depend on the chemical structure of doped site, thus C-N or C=N rich. It is due to the distribution of catalytic active site, defect, and bonding state. This result would be guide the direction of doping design of graphene based catalytic application.

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I23: Low dose STEM imaging of defects, sidegroups and organic molecules on graphene

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Suspended graphene sheets are the ultimately electron transparent and resilient support for atomically resolved low energy (60keV) scanning transmission electron microscopy (STEM) of entities, such as topological defects, side groups, or adsorbed molecules. Yet, conventional direct imaging is severely challenged by the dynamics under the probing electron beam. We circumvent the dose limitation by automated low-dose mapping of large sample areas covering several square microns, containing

random mixtures of such entities. Then we apply a maximum likelihood reconstruction [1,2], and retrieve effective high dose and low noise views of all the different entities. This powerful approach pushes the limits of atomically resolved electron microscopy into the realm of single molecules.

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I24: Novel BaC8 dopant pattern on graphene: interface effects and electron-phonon coupling.

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In this work the adsorption of Ba atoms on quasi-free-standing single-layer graphene has been studied for the first time. Doping of graphene with Ba leads to new adsorbate phase with BaC₈ stoichiometry and a well-defined interface structure with a novel $p(2\times 2)$ surface reconstruction. This structure is only observed in the monolayer case and different from the $p(\sqrt{3}\times\sqrt{3})\text{-R}30^\circ$ that is usually observed in the BaC₆ graphite intercalation compound. Also it was shown that the structure of the interface depends on the substrate resulting in Ba intercalation in case of an Au substrate and adsorption on top of graphene in the case of a Ge substrate. Using angle-resolved photoemission spectroscopy, we determine the full electronic structure of Ba doped graphene and find that graphene has a gapless spectral function for both substrates, as expected for the $p(2\times 2)$ adsorbate pattern. However it was shown that the doping level strongly depends on the substrate and is much higher in case of Au. These experimental results are in a good agreement with DFT modeling. We also observed “kinks” in band dispersion of Ba-doped grapheme, which stem from strong electron-phonon coupling. Using high-resolution angle-resolved photoemission spectroscopy and self-consistent analysis procedure we extracted Eliashberg functions and constants of electron phonon coupling for both substrates. Experimental data are in a good agreement with DFT modeling of these systems, showing higher coupling strength for Ge substrate, which in its turn increases temperature of superconducting transition. These results can be explained by higher doping level and softening of phonon modes on semiconducting substrate. Our study clarifies the important role of the number of layers and the substrate for the search of new electron-phonon coupling materials based on doped graphene layers.

I25: Optoelectronic properties of densely aligned suspended graphene nanoribbons array

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Graphene nanoribbons (GNRs) combine the unique electronic, optical and spin properties of graphene with a transport gap, which makes them an attractive candidate material for the channels of next-generation transistors. Up to now, we developed a novel method based on the advanced plasma CVD method [1] with nano scale Ni catalyst (Ni nanobar) for directly fabricating suspended GNRs devices [2]. In this study, we focused on the optoelectronic properties of suspended GNR. Firstly, we measured the photoresponse from the isolated very narrow (width: sub 10 nm) single suspended GNR prepared by plasma CVD at various temperatures (15~300 K) with the solar simulator illumination. As a result, single GNR sample recorded the relatively high photoresponsivity (~1000 A/W) at 30 K. Furthermore, the optoelectronic properties can significantly increase with the large scale suspended GNRs array, where over 1,000,000 of suspended GNRs are integrated. These results can contribute to developing the novel type optoelectronic applications with suspended GNR array in large scale.

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I26: Probing interface interaction in 2-dimensional materials and their heterostructures

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2-dimensional (2D) homo-/hetero-structures built up from layered materials have received growing attention owing to their simple fabrication, straightforward stacking and various types of band alignments. Optical and electrical properties have been investigated intensively to probe the interface coupling in 2D homo-/heterostructures. The mechanical interface interaction, however, has yet to be well studied. Here I will show two approaches, nanoindentation and surface plasmon enhanced Raman scattering, to probe effective modulus and local strain in 2D homo-/hetero-structures, respectively. Both results reflect the weak interlayer interaction in 2D layered structures. First, nanoindentation experiments indicate that the effective 2D modulus of a bilayer structure is lower than the sum of 2D modulus of each layer due to the interlayer sliding. Second, by coating 2D structures with silver or gold nanoparticles, the local strain existing at the metal-2D layer boundary will split the featured Raman peaks, but this splitting effect weakens as the number of layers increases because of the weak interlayer interaction. Our results not only provide mechanical insight to understanding interface interactions in 2D homo-/hetero-structures, but also potentially allow engineering of their properties as desired.

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I27: Scalable Processing of 2D Nanosheets into 3D Crumpled Nanoparticles

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3D Crumpled graphene was directly obtained from aqueous dispersions of pristine graphene using an industrially scalable spray drying technique. Capillary forces during the water evaporation induced the crumpling of nanosheets to multi-faced dimpled morphology. For the first time, the transition of 2D graphene nanosheets to a 3D crumpled morphology was directly observed inside the spray dryer. Graphene oxide (GO) was spray dried using the same procedure; however, their highly wrinkled final morphology was different than the crumpled pristine graphene nanosheets. The degree of crumpling of the nanosheets was controlled by changing the dimensionless ratio of evaporation rate to diffusion rate. Crumpled particles were redispersed into various solvents to evaluate their morphological changes as a response to rewetting. Crumpled GO nanosheets remained crumpled as a response to hydration, while the pristine graphene nanosheets unfolding behavior was solvent-dependent. This technique is similarly effective for dispersed inorganic nanosheets such as boron nitride and metal dichalcogenides. Crumpled graphene oxide may also be used as a precursor for the preparation of 3D networks (in both hydrogel and aerogel form) using a low-temperature sol-gel technique. The electrical conductivity of these samples is comparable to conductivity values reported for the networks prepared from native 2D graphene nanosheets.

I28: Single-walled carbon nanotubes and Buckminsterfullerene's in graphene stacks

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Single-walled carbon nanotubes (SWCNTs), Buckminsterfullerene's (C_{60}) and graphene belong to a family of low-dimensional carbon molecules. In this study, by using an aberration-corrected scanning transmission electron microscopy (STEM), we investigate hybrid structures made by sandwiching SWCNTs and C_{60} 's into a graphene stack. SWCNTs were deposited on monolayer graphene by using a floating catalyst chemical vapour decomposition (FC-CVD) reactor in combination with a thermal gradient assisted deposition and C_{60} 's by using a vacuum evaporation chamber. Subsequently, a sandwich structure was obtained by placing another monolayer of graphene on top of the deposited structures and adhered by introduction of a droplet of isopropyl alcohol. In this study we investigated four kinds of structures; **i)** C_{60} 's and **ii)** SWCNTs on a monolayer graphene and **iii)** C_{60} 's and **iv)** SWCNTs in a graphene sandwich. STEM investigations show that C_{60} 's in a sandwich structure are generally more stable than C_{60} 's on a monolayer graphene under the electron beam. The C_{60} 's in a graphene sandwich also show a well-ordered, periodic structure whereas those on a monolayer graphene without the sandwich exhibit more disorder. Different stacking orders of few layer C_{60} molecules were observed and identified as ABA and ABC close-packing by running STEM simulations. Finally, in this contribution we demonstrate a successful sandwiching of both individual and bundled SWCNTs in graphene stacks and discuss their collapsing behaviour.

I29: Spectroscopic studies of graphene molecules: Analysis of size and Crystallinity

Dervishi, Enkeleda (Los Alamos National Laboratory, Los Alamos, USA); Ji, Zhiqiang (Los Alamos National Laboratory, Los Alamos, USA); Hartmann, Nicolai (Los Alamos National Laboratory, Los Alamos, USA); Sykora, Milan (Los Alamos National Laboratory, Los Alamos, USA); Doorn, Steve (Los Alamos National Laboratory, Los Alamos, USA)

Graphene molecules are nanomaterials with interesting optical and electronic properties, making them promising candidates for a number of applications, such as photovoltaics, light-emission, bio-sensing and bio-imaging. In this work, we present a new synthetic approach for synthesis of graphene molecules with controlled morphological properties (armchair edges and controlled dimensions smaller than 2 nm). Even though, Raman studies of large-area graphene, as well as, nano-graphene sheets, with lateral dimensions larger than ~ 3 nm, have been previously reported, a thorough investigation of structures with well-controlled dimensions below 2 nm has been lacking. In this study, we present a detailed Raman analysis of graphene molecules with lateral dimensions between 0.76-1.39 nm, which correspond to structures with 16-79 ordered carbon rings. The samples were excited using laser light with two discrete wavelengths (405 nm and 532 nm), and their Raman spectral features, including integrated band area ratios and peak positions, were systematically investigated. Our studies indicated that the integrated area ratios of D and G bands (AD/AG) increase with the size of the molecules. The D and G band positions were also found to depend on the size of the graphene molecules. It is evident that the intensities of the double-frequency bands increase for both wavelengths, as the size of the graphene molecules increases. To elucidate the effect

of synthesis conditions on the structure of graphene molecule, we varied the reaction time and probed the crystallinity of the resulting graphene molecules. The integrated area band ratios and the band positions of the graphene molecules were strongly dependent on the reaction time. These comprehensive Raman studies can be used as a diagnostic tool for structural characterization and reaction dynamics of graphene molecules smaller than 2 nm, which is currently missing from the studies of larger graphene structures.

I30: Vertically Stacked Heterostructure With Low-Dimensional Nanomaterials

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Improving the integration level is important to both semiconductor industry and nanotechnology. The fabrication of nanoscaled devices is still a big challenge for conventional microfabrication process. Low-dimensional nanomaterials bring opportunities to the integration level improvement. Vertically-stacked devices with 2D materials utilize the vertical dimension to the utmost, as the devices function is realized within a ultra-thin layer. But scaling down the in-plane device size remains a problem. Here, we utilize 1D and 2D materials to construct vertical FETs. The introduction of 1D material greatly improves the in-plane integration level. The devices have high on/off ratio and large current density, and it can possibly be used to build logic circuit with high integration level. The vertical heterostructure can also be used as light detectors with high spatial resolution in future.

POSTER SESSION J: Non Carbon Materials

J1: Doping and interlayer interaction in h-BN monolayer and bilayer sheets

Saito, Susumu (Tokyo Institute of Technology, Meguro-ku, Tokyo, JPN); Fujimoto, Yoshitaka (Tokyo Institute of Technology, Meguro-ku, Tokyo, JPN)

We study pristine and C-doped monolayer and bilayer hexagonal BN sheets (h-BN) within the framework of the density-functional theory. We first show that the C doping at B and N sites in the monolayer h-BN sheet induce rather deep donor and acceptor states, respectively. We next show that biaxial tensile strain can reduce the ionization energies of both donor and acceptor states. More interestingly, in the case of the donor state, not only tensile but also compressive strain can reduce the ionization energy due to the interchange of the conduction band state to the nearly free electron state. Finally, we show that, in the case of bilayer h-BN sheet, the interlayer interaction can also reduce the ionization energy of donor state. Importantly, this reduction of the ionization energy is found to be enhanced by either uniaxial strain perpendicular to the sheet or biaxial tensile strain parallel to the sheet. These various ways to modify the electronic properties of h-BN sheets shown in the present work clearly indicate that h-BN sheets should be an important wide-gap semiconductor material for future device applications.

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J2: Investigation of round-shaped MoS₂ grown by chemical vapor deposition

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Molybdenum disulfide (MoS₂) crystals grown by chemical vapor deposition (CVD) are usually triangular or hexagonal geometries. However, round-shaped MoS₂ can be synthesized by atmospheric-pressure chemical vapor deposition in a sulfur-rich environment. We deposit MoS₂ on SiO₂/Si substrates using MoO₃ and S powder as precursors. A typical growth temperature is 850°C and Ar is used as carrier gas. Sizes of round-shaped MoS₂ range from a few micrometers to over one hundred micrometers in diameter, which depend on growth time. Raman spectrums show that round-shaped MoS₂ crystals also have characteristic Raman peaks at 384.0 and 402.8 cm⁻¹, which is just the same as triangular monolayer MoS₂. Atomic force microscopy (AFM) confirms round-shaped monolayer MoS₂ thickness to be about 1nm and indicates that round-shaped MoS₂ crystals are monolayer. We fabricate round-shaped MoS₂ FETs which have similar performance to triangular MoS₂ FETs.

J3: Controlling Catalyst Bulk Reservoir Effects for Monolayer Hexagonal Boron Nitride CVD

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Hexagonal boron nitride (h-BN) is an atomically-thin insulator with highly interesting properties as barrier-, spacer- or support-layer for future integrated electronics and photonics. Catalytic chemical vapor deposition (CVD) has emerged as the most promising route towards 'electronic-grade' h-BN films owing to its ability to produce high-quality layers over large areas, while being scalable and cost-effective. To date, h-BN CVD has been demonstrated on a range of polycrystalline metal foils and films, however, with the limited understanding of the underlying growth mechanisms under realistic processing conditions, growth control remains rudimentary. Here, we elucidate the key role of the catalyst bulk reservoir in the Fe-catalyzed CVD of h-BN [1]. Our comparative study of Fe foils annealed in either H₂ or NH₃ prior to growth demonstrates that the preannealing atmosphere strongly alters the Fe bulk phase evolution and subsequent B/N uptake mechanisms during precursor exposure, which in turn determines the coverage, thickness and uniformity of h-BN domains. Using in situ XRD and in situ XPS, we monitor the structural and chemical changes induced by the reaction atmosphere and rationally engineer a prefilled Fe catalyst to achieve better growth control. We show that NH₃-preannealed Fe foils enable growth of uniform monolayer h-BN, due to a N bulk-filling effect, which limits B and N diffusion into the catalyst during exposure to borazine and reduces the incubation time for h-BN nucleation. These effects act to minimize isothermal multilayer growth and suppress additional layer formation on cooling. We thus highlight the critical and controllable contribution of the catalyst bulk in CVD-based synthesis, providing a general growth rationale that can be applied to the wider class of layered compound materials. The catalyst bulk filling method presented here provides an elegant alternative to using different catalysts or using catalyst alloying [2] to control the solubility and permeability of the growth species.

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J4: Enhanced Photocatalytic Performance of Nano-kaolinite Prepared via Intercalating Method for Degradation of Rh-B under UV Light

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Hexagonal nano-kaolinite was successfully exfoliated via intercalation method. Several intercalating agents such as potassium and sodium acetate, hydrazine hydrate, and potassium nitrate were studied. The resulting materials were characterized using various techniques such X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field emission-scanning electron microscope (FE-SEM), transition electron microscope (TEM), BET, photoluminescence (PL), BET surface area and UV-visible. The XRD patterns shows that the characteristic peaks of kaolinite at $2\theta = 12.3^\circ$, 20.3° , 24.9° were observed. TEM and FE-SEM images show obviously a variety of morphologies, including platy, particles, booklets or sheets stacks and elongate of hexagonal kaolinite depending on the kind of the intercalating agents. FT-IR bands display a represented band for nitrogen doping in some samples. Moreover, the data obtained from PL of the produced materials revealed that the most interested sample has the highest intensity is due to the high density of electrons that attributed to the free electrons on nitrogen atom which was detected in FTIR analysis. Surface area and band gaps are also investigated. The promising nano-kaolinite was studied for degradation of Rhodamine B dye (Rh-B) under UV light. The results revealed that a complete degradation were takes place. Several parameters for degradation such as PH, concentration of Rhodamine B dye, catalyst dose and catalyst recycling are also investigated.

J5: Giant quantum-confined Stark effect in monolayer transition metal dichalcogenides

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Optical properties of monolayer transition metal dichalcogenides (TMDCs) are attracted attention due to their quantum-confined structure. Particularly, observation of the trion at room temperature is a solid evidence of the strong confinement effect. In recent studies, optical properties of monolayer TMDCs based on the electric field or the charge carrier modulation spectroscopy are well reported [1]. However, the effect of electric field is still not understood well [2]. This work provides a direct evidence of a giant quantum-confined Stark effect in monolayer TMDCs. We fabricated an electric double layer capacitors (EDLCs) using monolayer WS₂ and MoS₂, that were synthesized by chemical vapor deposition methods on mechanically exfoliated graphite [3]. As a dielectric material, we spincoated ion gel which is the mixture of ionic liquid ([EMIM][TFSI]) and tri-block co-polymer (PS-PMMA-PS). Using these devices, we observed PL spectral redshift (~ 10 meV) and the applied electric field is approximately $\sim 8 \times 10^6$ V/cm. Importantly, the redshift is proportional to square of applied voltages, V_G , which is a direct evidence of the quantum-confined Stark effect. Based on the great successes in PL measurements, as an additional step, we fabricated light-emitting diodes based on electric double layer for observation of

EL spectra. Two electrodes were deposited on mechanically exfoliated monolayer WSe₂ and the ion gel was spincoated on it. We successfully observed EL spectral due to excitons and trions. Very importantly, as observed in PL, EL spectra also revealed the quadratic VG dependent redshift because of the quantum confined Stark effect. Particularly, the maximum redshift in trion peaks was approximately 40 meV, which is close to the champion record in GaAs quantum wells.

[1] A. M. Jones et al. *Nature Nanotech.*, 8, 634 (2013)

[2] K. Matsuki et al. *Jpn. J. Appl. Phys.* accepted

[3] Y. Kobayashi, S. Sasaki, Y. Miyata et al. *ACS NANO*, 9, 4056 (2015)

J6: Semiconductor Nanotube In Non-Uniform Static Magnetic Field

Harutyunyan, Volodya (Russian-Armenian University, Yerevan, ARM)

Research in the field of semiconductor nanotubes (SNTs) has been progressing into a mature subject with several highly interdisciplinary subareas such as nanoelectronics, biosensing, optoelectronics, et al. One of the most powerful methods of influence on the states of charge carriers in SNTs, are the external static fields [2]. In this report we examine theoretically the effect of inhomogeneous static magnetic field on the states of charge carriers in SNT. A circular current loop is considered in the capacity of the source of an inhomogeneous magnetic field. It is shown that the magnetic field creates a new confining potential along the axis of the symmetry of nanotube. Using the variation approach, we obtain a description for the ground and first excited states of motion of the charge carriers along the symmetry axis. It is shown that in the presence of a nonuniform magnetic field a definite correlation takes place between the orbital motion of the particle in the cross section of the tube and the movement along the symmetry axis of SNT. The interband and intraband-intersubband magneto-optical transitions in SNT are also considered. The absorption is strictly resonant. In the case of interband transitions the presence of a magnetic field leads to an adjustable narrowing of the band gap of sample. The selection rules by the azimuthal quantum number are again caused by correlations between the orbital motion and the quantized motion of charge carriers along the symmetry axis. Both in the cases of interband and intraband magneto-optical transitions the threshold of absorption is shifted toward longer wavelengths.

J7: Theoretical Study on the Metal-Insulator Control by Atomic Adsorption onto the MXene dioxide Ti₂CO₂

Ando, Yasunobu (Department of Materials Engineering, The University of Tokyo, Tokyo, JPN); Watanabe, Satoshi (Department of Materials Engineering, The University of Tokyo, Tokyo, JPN)

Atomic-layer materials like graphene, silicene, germanene, and transition metal dichalcogenides has received great attention because of their potential use in various types of next-generation electronic devices. In 2011, a new, large family of atomic layer material; called MXenes (M_{n+1}X_n) synthesized from MAX phases (M_{n+1}A_nX_n) was reported. More than 60 compounds are known to host MAX phases. Therefore, MXenes have attracted increasing attention as promising candidates for new types of

atomic-layer materials. However, previous studies for applications of MXenes focused only on the suitability for energy devices such as Li-ion batteries and did not discuss the possibility of switching, even though it is expected to open a new direction for application of MXenes in electronic devices instead of energy ones. Therefore, through first-principles calculations using density functional theory, we investigate the possibility of controlling the metal–insulator properties of the Ti₂C MXene dioxide Ti₂CO₂ by ion adsorption. Our simulation reveals that Ti₂CO₂ is insulating with an indirect band gap of 0.44 eV. Upon atomic adsorption of H, Li, or Na, Ti₂CO₂ becomes metallic. This metal–insulator change may be used to produce switching devices with a high on/off ratio and low energy consumption by controlling ionic movement, as in ion batteries.

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Program for Friday, August 12th 2016

09:00 - 09:45	Key Note Lecture: C. Bichara <i>Modelling the growth of Single Wall Carbon Nanotubes</i>
09:45 - 10:00	Contributed Talk: Jerry Bernholc <i>Computational Exploration and Design of Nanoscale Sensors and Devices</i>
10:00 - 10:15	Contributed Talk: Riichiro Saito <i>Circular Dichroism of Single Wall Carbon Nanotubes</i>
10:15 - 10:30	Contributed Talk: Yoshiyuki Miyamoto <i>Theory of UV to THZ light conversion using graphene nano-ribbons</i>
10:30 - 11:00	Invited Talk: Tobias Hertel <i>Optical Spectroscopy of Doped SWNTs</i>
11:00 - 11:30	Coffee Break
11:30 - 12:00	Invited Talk: Yuval Yaish <i>Automated circuit fabrication and direct characterization of carbon nanotubes vibrations - Optical imaging of CNTs</i>
12:00 - 12:15	Contributed Talk: Sebastian Heeg <i>Carbon nanotube encapsulated dye molecules probe surface-enhanced Raman scattering</i>
12:15 - 12:45	Invited Talk: Daniel Heller <i>Carbon Nanotube Photoluminescence for Biomedicine</i>
12:45 - 13:00	Contributed Talk: Adam Bushmaker <i>Single Ion Adsorption on Individual Isolated Single Walled Carbon Nanotubes</i>
13:00 - 13:30	Pack Lunch
13:30 - 13:45	Surprise
13:45 - 14:30	Conference Summary and Poster Awards
14:30 - 14:45	NT17 Announcement
15:00	Closing

FRIDAY

KN5: Modelling the growth of Single Wall Carbon Nanotubes

Bichara, Christophe (CINaM, Aix-Marseille University and CNRS)

In spite of recent progress in the synthesis of single wall carbon nanotubes (SWNT) by catalytic chemical vapor deposition (CCVD), and the rise of commercially viable applications, a full control and understanding of property-selective growth still appears elusive. High synthesis temperatures, nano-metric sizes and the large number of correlated growth parameters involved, make the experimental investigation of growth mechanisms specially challenging. Theoretical approaches are not any easier, but I will show that dedicated computer simulations, including tight binding models [1], as well as DFT-based calculations, can provide useful insights. Different aspects have been investigated, in the case of Ni, taken as a prototypical catalyst, as well as other metals. Our discussion starts with the complex stability pattern of atomic carbon dissolved in subsurface layers of crystalline Ni that depends on the presence of a graphene surface layer [2]. For catalyst nanoparticles below 3 nm, relevant in the context of CCVD growth, the presence of carbon dissolved in surface layers induces a gradual melting at temperatures well below the melting temperature of pure nanoparticles of the same size. Calculated size dependent phase diagrams for Ni-C nanoparticles [3] indicate that faceted crystalline nanoparticles are unlikely to be observed in this size range under growth conditions. This raises the question of the role of the carbon dissolved in the catalyst during growth that is found to have a strong influence on the wetting properties of the metal-SWNT interface [4]. Through careful Transmission Electron Microscopy observations [5], so called tangential and perpendicular growth modes have been identified. Computer simulations are used to analyze these growth modes at the atomic scale, demonstrating that the tangential mode corresponds to a weak carbon supply and slow growth, while the perpendicular mode is observed when the carbon fraction in the nanoparticle is larger [6]. Growth experiments designed to tune the carbon fraction in the nanoparticle by changing the carbon feedstock (CO or CH₄) confirm this analysis. Finally we discuss the role of the different contributions to the stability and dynamics of the nanotube/nanoparticle interface on the possibility of a chiral selectivity.

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CT23: Computational Exploration and Design of Nanoscale Sensors and Devices

Bernholc, Jerry (NC State University, Raleigh, USA)

Carbon nanotubes are highly promising for chemical and biological sensing applications, owing to their high chemical and mechanical stabilities, high surface areas and unique electronic properties. We describe the results of extensive ab initio studies of the mechanisms of detection of small molecules: ammonia, nitrogen dioxide, glucose and ethylene, and simulations of nano circuits involving a nanotube functionalized with a fragment of polymerase I enzyme. The nano circuit monitors replication of a single-stranded DNA and can potentially be used to sequence DNA by detecting electrical signatures of the adding bases. We discuss modifications that should enable reliable distinction between some of the bases, and our work towards complete sequencing. If time permits, we will also discuss computational optimization of nanoribbon-based transistor structures with BN insulating layers and Al gate.

In collaboration with Y. Li, M. Hodak, W. Lu, and E. Briggs.

CT24: Circular Dichroism of Single Wall Carbon Nanotubes

Saito, Riichiro (Tohoku University, Sendai, JPN); Sato, Naomichi (Tohoku University, Sendai, JPN); Tatsumi, Yuki (Tohoku University, Sendai, JPN)

Recently, single wall carbon nanotubes (SWNTs) can be purified into not only a single chirality specified by two integers (n,m) but also left or right handedness of a SWNT (or enantiomers). Depending on handedness of the purified SWNTs, Kataura et al. and other group have showed that circular dichroism (CD) appears as a function of wavelength. For left and right handed single chirality SWNT, they show that (1) the sign of CD values alternate plus and minus as a function of the wavelength at Eii energy positions and that (2) at the same Eii, the opposite signs of the CD values appear for left and right handed SWNTs.

In this paper, we present a new theory for CD especially for SWNTs. The effect of CD is defined by the different optical absorption of a material for incident left and right circular lights. CD can be generally observed by molecules that have enantiomers. If we simply use the conventional theory of CD for molecules, the calculated CD values gives zero since the CD value that is integrated around the K point in the Brillouin zone exactly cancels that around the K' point due to the time-reversal symmetry for the electronic structure. This time-reversal symmetry is very robust for any possible lattice deformation and thus conventional theory for CD does not work at all. In the present work, however, a new formalism beyond so-called dipole approximation works well for obtaining the CD values of SWNTs. The analytic and numerical results of the CD values well reproduce the above experimental results. Thus we believe that this work gives an important step for understanding chirality dependent optical properties especially for SWNT enantiomers.

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CT25: Laser-decomposition of water enhanced by graphitic materials

Miyamoto, Yoshiyuki (JPN); Zhang, Hong (JPN); Cheng, Xinlu (JPN); Rubio, Angel (ZZZ)

Water decomposition is one of promising ways for production of hydrogen fuel which can be alternative to current fossil fuel for saving environment. We have studied water decomposition with short laser pulse (FWHM=10fs, 800nm) by performing the molecular-dynamics simulation combined with the time-dependent density functional theory. The simulation gave the threshold intensity of the laser E-field as 9 V/Å for an isolated water molecule, which is reduced into 6 V/Å when water molecules are above either graphene or above hBN, and reduced into 7 V/Å when water molecules are above gC₃N₄. In this presentation, we will discuss possible mechanisms of the reduction of threshold intensity of laser E-field and potential applications.

This work was supported by Science of Atomic Layers (SATL), Grant-in-Aid for Scientific Research for Innovative Areas by MEXT, Japan.

IT10: Optical Spectroscopy of Doped SWNTs

Hertel, Tobias (Julius-Maximilians-University, Wuerzburg, GER)

Chemical modification and doping of semiconducting carbon nanotubes plays an important role in tailoring their electronic and optical properties for applications. However, the assessment of doping levels and the associated changes of the electronic structure of SWNTs continues to present challenges for both, theory and experiment. Here we have investigated the photophysical properties of chemically and of gate-doped semiconducting single-wall carbon nanotubes (s-SWNTs) using stationary and femtosecond time-resolved spectroscopy, at the single-particle and at the ensemble levels. We compare the effects of different doping schemes on exciton- and trion-photophysics as well as for energy transport and dissipation. We also discuss the implications for different approaches to quantifying doping by optical means.

IT11: Automated circuit fabrication and direct characterization of carbon nanotubes vibrations - Optical imaging of CNTs

Yaish, Yuval (Andrew and Erna Viterbi Faculty of Electrical Engineering, Haifa, ISR)

Since their discovery carbon nanotubes (CNTs) have fascinated many researchers due to their unprecedented electrical, optical, thermal, and mechanical properties. Recently, a complete computer based on CNT circuits has been demonstrated. However, a major drawback in utilizing CNTs for practical applications is the difficulty in positioning or growing them at specific locations or in locating them on the substrate such that the circuit can be built around them. Here we present a simple, rapid, non-invasive, and scalable technique that enables optical imaging of CNT¹. Instead of relying on the CNT chemical properties to bind marker molecules we rely on the fact that the CNT is both a chemical and physical defect on the otherwise flat and uniform surface. Namely, it may serve as a seed for nucleation and growth of small size, optically visible, nano-crystals. As the CNT surface is not used to bind the molecules they can be removed completely after imaging, leaving the surface intact and thus the CNT electrical and mechanical properties are preserved. The successful and robust optical imaging allowed us to develop a dedicated image processing algorithm through which we are able to demonstrate a fully automated circuit design resulting in field effect transistors and inverters. Moreover, we demonstrate that this imaging method allows not only to locate CNTs but also, as in the case of suspended ones, to study their dynamic mechanical motion. The decorated tubes exhibit linear as well as non-linear Duffing type behavior, and for the first time transition from hardening to softening is observed.

[1] G. Zeevi, M. Shlafman, Y. E. Yaish et al, Nature Communications, 2016 (accepted)

CT26: Carbon nanotube encapsulated dye molecules probe surface-enhanced Raman scattering

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Surface-enhanced Raman scattering (SERS) is the giant increase in the Raman signal of molecules by surface plasmons of metal nanostructures. Even after 40 years of SERS, quantifying enhancement and refining our understanding of the underlying mechanism is challenging: the exact location of a molecule in a SERS hotspot, the orientation of its transition dipole and chemical interactions with the metal remain impossible to control experimentally. Here we overcome these limitations by probing SERS with aligned-sexithiophene (6T) molecules encapsulated inside carbon nanotubes. The tubes (i) carry the 6T into SERS hotspots by directed dielectrophoretic deposition, (ii) render them chemically inert and (iii) simultaneously define and reveal their location and orientation. We access SERS enhancement with unprecedented accuracy, both experimentally and by simulations according to the electromagnetic theory (EM) of SERS. The experimental enhancement exceeds the calculated value by two orders of magnitude and – in the absence of chemical enhancement - calls for treating SERS beyond the EM approach, e.g. within perturbation theory, where the plasmon forms an integral part of the Raman process

IT12: Carbon Nanotube Photoluminescence for Biomedicine

Heller, Daniel (Memorial Sloan Kettering Cancer Center, New York, USA)

The real-time and spatially-resolved detection and identification of analytes in biological media present important goals for next-generation nanoscale probes and sensors. To this end, we employ the intrinsic near-infrared fluorescence of single-walled carbon nanotubes which is photostable yet sensitive to the immediate environment. To build biomedical technologies that employ carbon nanotube photoluminescence, a better understanding of the optical response, as well as new methods to measure it in biological systems, are needed. We have developed new imaging platforms to quantify nanotube emission, including a method to conduct photoluminescence excitation/emission spectroscopy on living samples. We synthesized carbon nanotube-based photoluminescent sensors to interrogate analytes and processes in living specimens, including mammalian cells, 3D tumor spheroids, and in vivo.

CT27: Single Ion Adsorption on Individual Isolated Single Walled Carbon Nanotubes

Bushmaker, Adam (The Aerospace Corporation, El Segundo, USA); Oklejas, Vanessa (The Aerospace Corporation, El Segundo, USA); Walker, Don (The Aerospace Corporation, El Segundo, USA); Hopkins, Alan (The Aerospace Corporation, El Segundo, USA); Chen, Jihan (The University of Southern California, Los Angeles, USA); Cronin, Stephen (The University of Southern California, Los Angeles, USA)

The detection of single ions has, for many years, been the domain of large devices such as the Geiger counter, and to date, there have been no studies investigating the effects of ions on materials and devices at the single-ion level, despite the widespread use of gaseous ions to modify material surface properties, for instance by corona discharge. Here, we report on single gaseous ion adsorption onto individual carbon nanotube field effect transistors, which, due to the severely restricted one-dimensional current path, experience discrete, quantized resistance increases of over two orders of magnitude [1]. Switching events were observed during exposure to lightly ionized nitrogen, helium, oxygen, argon and air. This is in contrast to single neutral atom adsorption detection techniques, which have shown only small, barely detectable responses. Only positive ions cause changes, by the mechanism of ion potential induced carrier depletion, which is supported by density functional and Landauer transport theory. Our observations reveal a new single-ion/CNT heterostructure with novel electronic properties, and demonstrate a powerful new system for studying ion adsorption dynamics at the single-ion level.

[1] Bushmaker, A. W. et al. Single-ion adsorption and switching in carbon nanotubes. *Nature Communications* 7 (2016).

Satellite Symposia

Saturday
August 13th 2016



CCTN16: 11th International Symposium on Computational Challenges and Tools for Nanotubes

CNBMT16: 7th Symposium on Carbon Nanomaterials Biology, Medicine & Toxicology

CNTFA16: 4th Carbon Nanotube Thin Film Electronics and Applications Satellite

GSS16: 7th Graphene and 2D Materials Satellite Symposium

MSIN16: 10th International Workshop on Metrology, Standardization and Industrial Quality of Nanotubes

11th International Symposium on Computational Challenges and Tools for Nanotubes	
9:00-9:05	Opening the Satellite
9:05-9:50	Key Note Lecture: Steven G. Louie
	<i>Novel Interaction Effects in Quasi 2D Materials: Concepts and Computational Challenges (S1-13)</i>
9:50-10:15	Invited Talk: Charlotte Vets
	<i>Thermodynamic screening of bimetallic catalysts for chirality controlled growth of carbon nanotubes(S1-16)</i>
10:15-11:00	Coffee Break & Poster Session
11:00-11:25	Invited Talk: Ludger Wirtz
	<i>Excitons and phonons in Transition Metal Dichalcogenides: Simulation of optical and vibrational spectroscopy (S1-2)</i>
11:25-11:50	Invited Talk: Mikito Koshino
	<i>Physics of incommensurate 2D crystals (S1-15)</i>
11:50-12:10	Contributed Talk: Florian Fuchs
	<i>Investigation of Carbon Nanotube Based Field-effect Transistors Using Atomistic Quantum Transport and Numerical Device Simulation (S1-10)</i>
12:10-12:30	Contributed Talk: Yoshiyuki Miyamoto
	<i>Laser-decomposition of water enhanced by graphitic materials (S1-11)</i>
12:30-13:00	Lunch
13:00-14:00	Poster Session 1
14:00-14:25	Invited Talk: Peter Blaha
	<i>Theoretical spectroscopy on Fullerenes (S1-5)</i>
14:25-14:50	Invited Talk: Takeshi Nakanishi
	<i>Effective-mass theory for collapsed carbon nanotubes and bilayer graphene with closed edges (S1-7)</i>
14:50-15:10	Contributed Talk: Igor Bondarev
	<i>Plasmon mediated charge transport theory for hybrid metal-semiconductor nanotube systems (S1-3)</i>
15:10-16:00	Coffee Break + Posters Session 2
16:00-16:25	Invited Talk: Masahiro Sakurai
	<i>Pressure-induced structural transformation of carbon nanotube solids into new crystalline phases and prediction of their electronic and optical properties (S1-4)</i>
16:25-16:50	Invited Talk: Roland Gillen
	<i>Assessing and improving the DFT+D3 method for van-derWaals interaction in layered materials (S1-1)</i>
16:50-17:00	Closings Remarks
17:00	Closing the Satellite

CCTN16: 11th International Symposium on Computational Challenges and Tools for Nanotubes

S1-1: Assessing and improving the DFT+D3 method for van-der-Waals interaction in layered materials

Gillen, Roland (TU Berlin, Berlin, GER)

The novel physics in two-dimensional and/or layered materials gave rise to a recent advent of scientific publications with a variety of proposed applications. One demand on a theoretical study of such materials is the proper inclusion of non covalent bonding effects between layers and/or adsorbed molecules to obtain the correct geometries and derived effects on the electronic and vibronic structures.

A flexible and controllable description of such van-der-Waals interactions can be achieved by a posteriori corrections of semi-local density functional theory (DFT) in the recently proposed DFT+D3 scheme [1]. Using a set of high-throughput pseudopotentials, we have assessed the performance of DFT-D3 for a range of layered and non-layered solids. Based on this assessment, we devised a simple fitting procedure and obtained a slightly altered set of parameters that led to further improvement of the predicted lattice constants and bond lengths compared to the originally proposed parameters.

The obtained geometries were used to simulate the optical spectra (including electron-hole effects) of mono-, bi- and trilayers of various transition metal dichalcogenides with hexagonal and orthorhombic crystal structures [2]. Results of these calculations will be presented.

[1] Grimme et al., *J. Comput. Chem.* 32, 1456 (2011).

[2] Gillen et al., *arXiv:1605.01972* (2016)

S1-2: Excitons and phonons in Transition Metal Dichalcogenides: Simulation of optical and vibrational spectroscopy

Wirtz, Ludger (University of Luxembourg, Luxembourg)

Transition metal dichalcogenides (TMDs) have excellent optical and electronic properties for nano-engineering applications. Optical absorption and luminescence spectra are dominated by strong excitonic effects. In particular, resonant Raman spectroscopy is a very complete characterization tool that provides information about the vibrational modes and the optical spectrum in the same experiment: when the laser energy is close to an electronic transition, the scattered light intensity is increased due to resonance with an electronic transition.

We present first an overview [1] over the state-of-the-art of theoretical spectroscopy of TMDs. Ground-state and vibrational properties are calculated with density-functional theory. Optical absorption spectra are obtained using GW corrections to the band structure and the Bethe-Salpeter equation to include excitonic effects. Spin-orbit interaction is explicitly included in all calculations [2]. Using a quasi-static finite differences approach [3], we calculate the dielectric susceptibility for different light polarizations and different phonon displacements in order to determine the Raman

tensor of TMDs, in particular of multi-layer and bulk MoTe₂. We explain recent experimental results for the splitting of high-frequency modes [4] where strong deviations of the Raman intensities from the non-resonant Raman model were observed. We furthermore discuss the effects of finite temperature on the optical spectra [5].

Collaborations with the authors of the references below are gratefully acknowledged.

[1] A. Molina-Sánchez, K. Hummer, L. Wirtz, *Surface Science Reports* 70, 554 (2015).

[2] A. Molina-Sánchez, D. Sangalli, K. Hummer, A. Marini, and L. Wirtz, *Phys. Rev. B* 88, 045412 (2013).

[3] Y. Gillet et. al., *Phys. Rev. B* 88, 094305 (2013).

[4] G. Froehlicher, E. Lorchat, F. Fernique, C. Joshi, A. Molina-Sánchez, L. Wirtz, and S. Berciaud, *Nano Lett.* 15, 6481 (2015).

[5] A. Molina-Sánchez, M. Palummo, A. Marini, and L. Wirtz, *Phys. Rev. B* 93, 155435 (2016).

S1-3: Plasmon mediated charge transport theory for hybrid metal-semiconductor nanotube systems

Bondarev, Igor (North Carolina Central University, Durham, USA); Gelin, Maxim (TU Munchen, Munich, GER)

We develop a quantum theory for plasmon mediated charge transport in hybrid metal-semiconductor nanotube systems composed of semiconducting single wall carbon nanotubes (CNs) that encapsulate metallic atomic wires (AWs) of finite length [1]. Encapsulating metallic wires of just one atom thick into a single wall CN, metallic or semiconducting, is known to drastically alter the transport properties of the compound hybrid system. For example, metallic single wall CNs encapsulating europium AWs exhibit extra conduction channels to supplement an overall “Tomonaga-Luttinger liquid”-like transport behaviour [2]. For hybrid metal-semiconductor systems we report on, an interesting feature is that their conductance inside the CN forbidden gap is contributed by the AW alone, while also being affected by near-fields of nanotube plasmons. Our plasmon mediated charge transport theory is built on the matrix Green’s functions formalism by Mujica, Kemp and Ratner [3], which is exact in the limit of low temperature and small external bias applied. Our theory and numerical simulations predict generic Fano resonances in charge transfer through the system, whereby the AW-CN near-field interaction blocks some of the pristine AW transmission band channels to open up new coherent channels in the CN forbidden gap outside the AW transmission band. This effect can be used to optimize charge transfer in hybrid nanodevices built on metal-semiconductor nanotube systems.

I.V.B. is supported by the US Department of Energy (DE-SC0007117). M.F.G. is partly supported by the US National Science Foundation (ECCS-1306871).

[1] M.F.Gelin and I.V.Bondarev, *Phys. Rev. B* 93, 115422 (2016).

[2] R.Nakanishi, R.Kitaura, P.Ayala, H.Shiozawa, K.de Blauwe, P.Hoffmann, D.Choi, Y.Miyata, T.Pichler, and H.Shinohara, *Phys. Rev. B* 86, 115445 (2012).

[3] V.Mujica, M.Kemp, M.A.Ratner, *J. Chem. Phys.* 101, 6849 (1994); *ibid.* 101, 6856 (1994).

S1-4: Pressure-induced structural transformation of carbon nanotube solids into new crystalline phases and prediction of their electronic and optical properties

Sakurai, Masahiro (The University of Texas at Austin, Austin, Texas, USA)

We have studied the pressure-induced structural transformation of carbon nanotube solids by performing constant-pressure molecular-dynamics (MD) simulations combined with the transferable tight-binding model for carbon [1,2]. In this talk, we report that carbon nanotube solids under pressure are predicted to exhibit a rich variety of structural transformations into nanostructured carbon phases. In particular, crystalline phases obtained in the MD simulations are found to include two kinds of hexagonal diamond polymorphs and a fourfold coordinated phase in the body-centered tetragonal structure. We also present the electronic and optical properties of the predicted diamond polymorphs using the GW approximation method and the GW plus Bethe-Salpeter equation approach [3]. This work is done in collaboration with Profs. S. Saito and S. G. Louie.

[1] M. Sakurai and S. Saito, *Jpn. J. Appl. Phys.* 49, 02BB05 (2010).

[2] M. Sakurai and S. Saito, *Physica E* 43, 673 (2011).

[3] M. Sakurai, S. Saito, and S. G. Louie, in preparation.

S1-5: Theoretical spectroscopy on Fullerenes

Blaha, Peter (Materialchemie, TU Vienna, Vienna, AUT)

Most theoretical calculations of solids are nowadays based on Density Functional Theory (DFT). However, DFT is a theory of the ground state and application to excited states is in principle not justified. Nevertheless it is common practice to use the resulting single particle eigenvalues and wave functions of a DFT calculation also for the interpretation of spectroscopies like XANES, ELNES or XPS. I will describe XANES K-edge calculations on various fullerenes based on our bandstructure code WIEN2k [1], where we model the excited states explicitly by more or less sophisticated approaches like core-holes and Slater's transition state all the way to many-body perturbation techniques like GW and BSE.

[1] <http://www.wien2k.at>

S1-6: Vibrational properties of isotopically controlled carbon nanotubes

Saito, Susumu (Tokyo Institute of Technology, Meguro-ku, Tokyo, JPN); Bando, Yuki (Tokyo Institute of Technology, Meguro-ku, Tokyo, JPN)

We study the vibrational properties of carbon nanotubes composed of alternating regions of ^{12}C and ^{13}C stacked along the tube-axis direction. This kind of "isotopic superlattices" utilizing ^{12}C and ^{13}C regions has already been synthesized in the case of diamond and, interestingly, carrier confinement in ^{12}C regions is found to take place. The strong electron-phonon interaction in covalent carbon materials and the sizable isotopic mass ratio of 13/12 are considered to be responsible for the interesting electronic behavior in isotopic superlattice, and are expected to realize interesting electronic properties in isotopically controlled carbon nanotubes as well. In the present work we address the vibrational properties of isotopically controlled carbon

nanotube which is of fundamental importance in predicting their electronic properties in the future. We combine the density-functional perturbation theory with the inverse Fourier transformation to calculate the force-constant matrix of the isotopically controlled carbon nanotubes, and realize the first-principles calculation of the dynamical matrix and therefore the vibrational properties of the isotopically controlled carbon nanotubes with very large unit cell. We especially analyze the radial breathing modes in detail.

S1-7: Effective-mass theory for collapsed carbon nanotubes and bilayer graphene with closed edges

Nakanishi, Takeshi (AIST, Tsukuba, JPN)

We theoretically study effects of inter-wall interaction in collapsed carbon nanotubes, first directly calculating effective inter-wall interaction within an effective-mass scheme and second regarding collapsed tubes as ribbons of bilayer graphene with closed edges described by boundary conditions explicitly derived.¹ Within the effective-mass scheme, effects of inter-wall interactions are shown to be important in non-chiral nanotubes such as zigzag and armchair. In fact, with the increase in the width of the flattened region, the band structure approaches that of a bilayer ribbon in which the electron motion in the ribbon-width direction is discretized. For zigzag and armchair nanotubes, the same results can be derived by calculating boundary conditions corresponding to the closed-edge structure in which the top and bottom layers are smoothly connected through a monolayer graphene. Effects of the closed-edge are shown, including band gap opening for the bilayer graphene in AB stacking, and chiral states, when armchair nanotubes are collapsed into AA or AA' stackings. In chiral nanotubes, inter-wall interaction can essentially be neglected except in the vicinity of non-chiral tubes. Inter-wall interactions diminish rapidly when chiral angle deviates from zigzag or armchair, although the decay is slower in the vicinity of the armchair tube.

[1]. T. Nakanishi and T. Ando, Phys. Rev. **B 91** (2015) 155420.

S1-8: Improved recursive Green's function formalism for defective carbon nanotubes

Teichert, Fabian (Dresden Center for Computational Materials Science (DCMS), Dresden, GER); Zienert, Andreas (Center for Microtechnologies (ZfM), TU Chemnitz, Chemnitz, GER); Schuster, Jörg (Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, GER); Schreiber, Michael (Institute of Physics, TU Chemnitz, Chemnitz, GER)

A new and very efficient approach for calculating the electron transport in arbitrary carbon nanotubes (CNTs) with randomly positioned defects is described. CNTs of realistic size up to several microns with up to thousands of defects can be treated with this method.

During any step of the device fabrication, defects are introduced to all CNT devices fabricated so far, even under best laboratory conditions. Nevertheless, most of the theoretical studies deal with ideal CNTs, not taking the influence of defects into account. The difficulty of electronic transport calculations in this context is that

defective systems contain a huge number of atoms. This makes the usage of density functional theory (DFT), which scales cubically with the number of atoms, unpractical. Thus, the development and improvement of theoretical methods is an important task to overcome the system size limitations.

We present our new and very efficient approach. The electronic structure is described by a hybrid model which uses the fastness of the tight binding approach as well as the good accuracy of DFT. The transport calculations are performed within the common quantum transport theory in combination with a fast, linearly scaling recursive Green's function formalism (RGF). This allows us to treat large systems quantum-mechanically. We further show our algorithm, which accelerates the common RGF, using the iteration steps of the renormalization decimation algorithm. This leads to a smaller effective system. The computational complexity scales linearly with the number of defects, instead of linearly with the total system length for the conventional approach. We show that the scaling of the calculation time of the Green's function depends on the defect density. Furthermore, we discuss the calculation time and the memory requirement of the whole transport formalism applied to defective carbon nanotubes. Finally, we show results concerning the conductance of CNTs with mono- and divacancy defects.

S1-9: Impurity invisibility in graphene: Symmetry guidelines for the design of efficient sensors

Ferreira, Mauro (Trinity College Dublin, Dublin)

Renowned for its sensitivity to detect the presence of numerous substances, graphene is an excellent chemical sensor. Unfortunately, which general features a dopant must have in order to enter the list of substances detectable by graphene are not exactly known. Here we demonstrate with a simple model calculation implemented in three different ways that one of such features is the symmetry properties of the impurity binding to graphene. In particular, we show that electronic scattering is suppressed when dopants are bound symmetrically to both graphene sub-lattices, giving rise to impurity invisibility. In contrast, dopants that affect the two sublattices asymmetrically are more strongly scattered and therefore the most likely candidates to being chemically sensed by graphene. Furthermore, we demonstrate that impurity invisibility is lifted with the introduction of a symmetry-breaking perturbation such as uniaxial strain. In this case, graphene with sublattice symmetric dopants will function as efficient strain sensors. We argue that by classifying dopants through their bonding symmetry leads to a more efficient way of identifying suitable components for graphene-based sensors.

S1-10: Investigation of Carbon Nanotube Based Field-effect Transistors Using Atomistic Quantum Transport and Numerical Device Simulation

Fuchs, Florian (Helmholtz-Zentrum Dresden Rossendorf, Dresden, GER); Zienert, Andreas (Center for Microtechnologies, Chemnitz, GER); Schuster, Jörg (Fraunhofer Institute for Electronic Nano Systems, Chemnitz, GER); Mothes, Sven (Chair for Electron Device and Integrated Circuits, Dresden, GER); Claus, Martin (Chair for Electron Device and Integrated Circuits, Dresden, GER); Gemming, Sibylle (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, GER)

Carbon nanotube based field-effect transistors (CNTFETs) are studied by using atomistic quantum transport simulation and numerical device simulation. Atomistic simulations are based on the non-equilibrium Green's functions formalism, where self-consistent extended Hückel theory is used¹. We apply a parameter set previously developed in our group to describe contacts between metals and carbon nanotubes with a density functional theory (DFT)-like accuracy². Numerical device simulations based on the effective-mass Schrödinger equation are done for comparison³ to highlight the strengths but also the limitations of this widely used method. The studied CNTFETs consist of n-doped source- and drain-electrodes together with an ideal wrap-around gate. Thus, the transistor exhibits Ohmic contacts and is comparable to the one studied experimentally by Lu et al.⁴.

Different CNTs with diameters ranging from 0.5 nm (7,0-CNT) to 1.3 nm (16,0-CNT) are compared. For larger diameters, band-to-band tunneling (BTBT) takes place, leading to ambipolar transfer characteristics. For small diameters, however, states within the channel are strongly localized and the BTBT is subsequently suppressed, resulting in very high on/off ratios of about 10^7 and ideal unipolar transfer characteristics. We investigate how different device parameters influence the device performance and show that the studied CNTFET shows excellent properties for channel lengths down to 8 nm. Finally, a comparison between the atomistic model and numerical device simulation is given. We show that the on- and off-currents are described in very good agreement and discuss the differences with respect to the switching behavior.

[1] Calculations performed using Atomistix ToolKit 12.8
(www.quantumwise.com)

[2] Zienert et al., *Nanotechnology* **25** (2014)

[3] Claus et al., *Journal of Computational Electronics* **13** (2014)

[4] Lu et al., *Journal of the American Chemical Society* **128** (2006)

S1-11: Laser-decomposition of water enhanced by graphitic materials

Miyamoto, Yoshiyuki (JPN); Zhang, Hong (JPN); Cheng, Xinlu (JPN); Rubio, Angel (ZZZ)

Water decomposition is one of promising ways for production of hydrogen fuel which can be alternative to current fossil fuel for saving environment. We have studied water decomposition with short laser pulse (FWHM=10fs, 800nm) by performing the molecular-dynamics simulation combined with the time-dependent density functional theory.

The simulation gave the threshold intensity of the laser E-field as 9 V/\AA for an isolated water molecule, which is reduced into 6 V/\AA when water molecules are above either graphene or above hBN, and reduced into 7 V/\AA when water molecules are above gC_3N_4 . In this presentation, we will discuss possible mechanisms of the reduction of threshold intensity of laser E-field and potential applications.

This work was supported by Science of Atomic Layers (SATL), Grant-in-Aid for Scientific Research for Innovative Areas by MEXT, Japan.

S1-12: Molecular Dynamics Growth of Chirality-Defined Carbon Nanotubes in Octopus Mode

Yoshikawa, Ryo (The University of Tokyo, Tokyo, JPN); Takagi, Yukai (The University of Tokyo, Tokyo, JPN); Ukai, Hiroyuki (The University of Tokyo, Tokyo, JPN); Chiashi, Shohei

(The University of Tokyo, Tokyo, JPN); Maruyama, Shigeo (The University of Tokyo, Tokyo, JPN)

Molecular dynamics (MD) simulations are often used to analyze the mechanism of carbon nanotube (CNT) growth¹. However, because CNTs grown in MD simulations were too defective, the mechanism of chirality-selection is almost never discussed despite experimental reports of chirality specific growth². We tuned the temperature and the free (gas phase) carbon density and successfully simulated several kinds of chirality-defined nanotube growth including (9, 0) from Fe catalyst, (14, 1) and (15, 2) from Co catalyst. They grew in octopus mode, characterized by carbon chains attached to the CNT edge on the surface of the catalyst, with kinks running along the zigzag edge. In addition, we developed Tersoff-type potential of bimetallic catalysts including Fe-Co, Cu-Co and W-Co. The chirality of nanotubes grown from these bimetallic catalysts in simulation will be discussed as well.

[1] Y. Shibuta and S. Maruyama, Chem. Phys. Lett., 382 (2003) 381.

[2] F. Yang, et al., Nature, 510 (2014) 522.

S1-13: Novel Interaction Effects in Quasi 2D Materials: Concepts and Computational Challenges

Louie, Steven G (University of California at Berkeley, Berkeley, USA)

Atomically thin quasi two-dimensional (2D) materials and their nanostructures can exhibit highly unusual behaviors. Owing to their reduced dimensionality, these materials present opportunities for manifestation of concepts and phenomena that may not be so prominent or have not been seen in bulk materials. Symmetry, many-body interaction, doping, and substrate screening effects often play a critical role in shaping qualitatively and quantitatively their properties, and thus their potential for applications. We present here theoretical studies on monolayer and few-layer transition metal dichalcogenides and metal monochalcogenides, as well as black phosphorus and other 2D crystals. Several phenomena are discussed: novel exciton behaviors; tunable transport, optical, magnetic, and plasmonic properties; and the dominant influence of substrate screening. This work was supported by the NSF and US Department of Energy.

S1-14: Optical spectra of strained carbon nanotubes: The origin of strain-induced shifts

Wagner, Christian (Technische Universität Chemnitz, Chemnitz, GER); Schuster, Jörg (Fraunhofer ENAS, Chemnitz, GER); Schreiber, Michael (Technische Universität Chemnitz, Chemnitz, GER); Schleife, André (University of Illinois at Urbana-Champaign, Urbana / IL, USA); Gessner, Thomas (Fraunhofer ENAS, Chemnitz, GER)

The integration of carbon nanotubes (CNTs) into microelectronic structures is feasible, nowadays. Therefore, sensors, e.g. optical sensors based on CNTs, are a recent research field for applied research. Under strain, a CNT opens or closes its

band gap – depending on its chiral angle. This property makes CNTs interesting for strain sensing at the nano scale.

Electronic structure calculations are required to model optical spectra of CNTs: We use independent-particle (density functional theory, DFT) and single-quasiparticle band structures (GoWo@LDA) to investigate the strain-dependence of the band gap. The Bethe-Salpeter equation (BSE) is applied for calculating optical spectra including excitonic effects. In a one-dimensional system, these calculations require truncations of the Coulomb interaction of periodic images in the supercell approach.

In order to disentangle the impact of the Coulomb truncation on the excitonic peaks in the optical spectrum, we apply different codes and approaches: In yambo [1], the microscopic screening matrix is generated and included in the BSE scheme – with and without Coulomb truncation. In a custom BSE implementation of VASP [2], the macroscopic dielectric constant is given as a static screening value and Coulomb truncation is not included. With this, different effects on the excitonic binding energy in CNTs can be separated. For example we can show that the binding energy scales with ε^{-2} – even in the case of Coulomb truncation, where the static dielectric constant ε is regularized.

We discuss the impact of the different approaches on the strain-induced peaks and derive empirical parameters in order to describe the peak shift. These parameters are useful for optical device modeling based on strained CNTs as well as CNT spectroscopy, e.g. infrared spectroscopy, and may allow extrapolation to other CNTs.

[1] A. Marini et al., Computer Physics Communications 180, 1392 (2009)

[2] F. Fuchs et al., Physical Review B 78, 085103 (2008)

S1-15: Physics of incommensurate 2D crystals

Koshino, Mikito (Tohoku University, Sendai, JPN)

Recent development in 2D materials realized unusual incommensurate systems in which the atomic layers are irregularly stacked without common lattice periods. There the long-period interference pattern of lattice structures completely modifies the physical properties. Here we report our theoretical studies on the various electronic properties in incommensurate 2D systems. We first introduce an effective-mass analysis to describe the low-energy physics, which can be applied to general incommensurate 2D systems, including twisted graphene bilayer, hexagonal-boron-nitride graphene composite system and also one-dimensional systems such as double-walled carbon nanotubes. [1,2,3]

We then show our recent work on the strain effect in moiré system. [4] When the moiré period is sufficiently long, the lattice of 2D system is automatically distorted to maximize the area of the preferred stacking structure. By using an appropriate phenomenological model for the interlayer interaction, we actually demonstrate a considerable distortion takes place in twisted graphene bilayer with smaller rotation angle (< 2 degree), and it significantly modifies the electronic band structure.

[1] Mikito Koshino, New J. Phys. 17, 015014 (2015).

[2] Pilkyung Moon and Mikito Koshino, Phys. Rev. B 90, 155406 (2014).

[3] Mikito Koshino, Pilkyung Moon and Young-Woo Son, Phys. Rev. B 91, 035405 (2015).

[4] Nguyen N. T. Nam and Mikito Koshino, unpublished.

S1-16: Thermodynamic screening of bimetallic catalysts for chirality controlled growth of carbon nanotubes

Vets, Charlotte (University of Antwerp, Department of Chemistry, Research group Plasmant, Wilrijk, BEL); Neyts, Erik (University of Antwerp, Department of Chemistry, Research group Plasmant, Wilrijk, BEL)

Chirality controlled growth of CNTs remains a topic of major importance [1]. Bimetallic catalysts provide a possible means to achieve better chirality control [2,3]. In this work, we investigate one of the factors potentially controlling chirality during CNT growth: the adsorption energy of a CNT on a bimetallic catalyst. We use Density Functional Theory (DFT) calculations in order to first investigate the stability of several catalyst nanoparticles (NPs), in terms of their cohesive energy and formation enthalpy. Six NP alloys are simulated in various compositions and atom distributions, both without and with interstitial carbons (to mimic the dissolution of carbon in the system [4,5]). Subsequently, we use Molecular Dynamics (MD) simulations to study the melting behaviour of a selection of stable NP alloys [6], as it has been shown that chirality control is more readily achieved at lower temperatures, in which case the NP is more likely to remain in the solid state [7]. Finally, we use DFT to calculate the adsorption energies of hydrogen-passivated CNTs with various chiralities on the selected stable NPs. This thermodynamic screening can provide insights in how to steer the preference for certain chiralities.

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- [2] Chiang, W.-H. et al. *ACS Nano* 3, 12, 4023-4032 (2009).
- [3] Silvearv, F. et al. *J. Mater. Chem. C* 3, 3422-3427 (2015).
- [4] Magnin, Y. et al. *Phys. Rev. Lett.* 115, 205502 (2015).
- [5] He, M. et al. *Nanoscale* 7, 20284-20289 (2015).
- [6] Neyts, E. C. et al. *J. Phys. Chem. C* 113, 2771-2776 (2009).
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7th Symposium on Carbon Nanomaterials Biology, Medicine & Toxicology	
9:00-9:05	Opening the Satellite
9:05-9:45	Key Note Lecture: Rui Peng <i>Graphene oxide and its derivatives: immunological effects and the application in cancer immunotherapy. (S2-2)</i>
9:45-10:15	Invited Talk: A. von dem Bussche <i>Linking nanomechanical mechanisms to carbon nanotube-induced toxicity (S2-12)</i>
10:15-10:50	Coffee Break & Poster Session 1
10:50-11:20	Invited Talk: Daniel Heller <i>Biometrology Enabled by Carbon Nanotube Optical Bandgap Modulation (S2-4)</i>
11:20-11:50	Invited Talk: Zhuang Liu <i>2D nanomaterials in Biomedicine: Graphene and Beyond (S2-10)</i>
11:50-12:10	Contributed Talk: Eri Hirata <i>The effect of carbon nanohorns on human monocyte and mesenchymal stem cells (S2-9)</i>
12:10-12:30	Contributed Talk: Takuya Ushiyama <i>Flexible carbon nanotube interdigitated electrode for electrochemical biosensors (S2-11)</i>
12:30-13:00	Lunch
13:00-14:30	Poster Session 2
14:30-15:00	Invited Talk: Silvia Marchesan <i>Functionalization of Carbon Nanostructures: how to play a winning game in the biomaterials field (S2-1)</i>
15:00-15:20	Contributed Talk: A. Boghossian <i>Engineering Bio-Wrappings for Optical Single-Walled Carbon Nanotube (SWCNT) Sensing Applications</i>
15:20-16:00	Coffee Break
16:00-16:30	Invited Talk: Peter Wick <i>Carbon based materials - a health perspective (S2-5)</i>
16:30-16:50	Contributed Talk: Laura Lagier <i>Compared ecotoxicity of carbon-based nanoparticles on <i>Xenopus laevis</i> tadpole (S2-6)</i>
16:50	Closing the Satellite

CNBMT16: 7th Symposium on Carbon Nanomaterials Biology, Medicine & Toxicology

S2-1: Functionalization of Carbon Nanostructures: how to play a winning game in the biomaterials field

Marchesan, Silvia (University of Trieste, Trieste, ITA)

Carbon nanostructures (CNS) have emerged as highly innovative nanomaterials for biological use, including the fields of drug delivery, regenerative medicine and even molecular detection. However, CNS typically suffer from high aggregation propensity in aqueous media, so that their appropriate functionalization becomes a must to tune their properties towards desired applications, whilst preserving their unique features. Here, we discuss how chemical functionalization of CNS is a crucial tool to deliver innovation. Examples will range from the application of CNS unique extended π -system electronic properties to connect cells of conductive tissue, to their incorporation into supramolecular hydrogel systems that gain self-healing ability. Using functionalized CNS thus holds great promise in providing innovative solutions to address key challenges in the fields of medicine.

S2-2: Graphene oxide and its derivatives: immunological effects and the application in cancer immunotherapy

Xu, Ligeng (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN); Xu, Jun (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN); Tan, Xiaofang (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN); Wang, Ting (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN); Xiang, Jian (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN); Feng, Liangzhu (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN); Liu, Zhuang (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, AUT); Peng, Rui (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN)

Graphene oxide (GO) and its derivatives have attracted great attention in biomedicine owing to their unique physicochemical properties. My group is currently working on the immunological effects of GO and its derivatives. Our recent work show that GO itself can induce multiple toll-like receptors (TLRs)-regulated inflammatory responses. Further coating the GO with polyethylene glycol (PEG) and/or various types of polyethylenimine (PEI) would vary the surface chemistry and therefore altering their immunological effects. Excitingly, compared with single-polymer modified GOs (GO-PEG and GO-PEI), certain dual-polymer modified GO (GO-PEG-PEI) can act as a positive modulator to promote the maturation of dendritic cells (DCs) and enhance their cytokine secretion through activation of multiple TLR pathways. Moreover, using urease B (Ure B, a specific antigen for *Helicobacter pylori*, which is a class I carcinogen for gastric cancer) as the model antigen, we demonstrate that this GO-PEG-PEI can serve as an antigen carrier to effectively shuttle antigens into DCs. These two advantages enable GO-PEG-PEI to

serve as a novel vaccine adjuvant. In the subsequent in vivo experiments, compared with free Ure B and clinically used aluminum-adjuvant-based vaccine (Alum-Ure B), GO-PEG-PEI-Ure B induces stronger cellular immunity via intradermal administration, suggesting promising applications in cancer immunotherapy. Although future work is required to further explore the molecular mechanisms behind these immunological effects, our work not only demonstrate the great promise of GO and its derivatives in novel vaccine nano-adjuvants and immunotherapy, but also highlight the critical roles of surface chemistry for the rational design of nano-adjuvants.

S2-3: Modulating single-walled carbon nanotube opto-electronic properties by chromophore confinement

Lahjiri, Fayçal (Laboratoire Charles Coulomb, Montpellier, FRA); Cassabois, Guillaume (Laboratoire Charles Coulomb, Montpellier, FRA); Izard, Nicolas (Laboratoire Charles Coulomb, Montpellier, FRA); Jusselme, Bruno (Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences, Gif-sur-Yvette, FRA); Campidelli, Stéphane (Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences, Gif-sur-Yvette, FRA); Saito, Takeshi (National Institute of Advanced Industrial Science and Technology, Tsukuba, FRA); Lauret, Jean-Sébastien (Laboratoire Aimé Cotton, Orsay, FRA); Delpont, Géraud (Laboratoire Aimé Cotton, Orsay, FRA); Bantignies, Jean-Louis (Laboratoire Charles Coulomb, Montpellier, FRA); Alvarez, Laurent (Laboratoire Charles Coulomb, Montpellier, FRA)

Opto-electronic properties of single-walled carbon nanotubes can be significantly modified by chromophore confinement into their hollow core. For instance, charge transfers are evidenced from Raman data analysis. First, by exciting nanotubes far from the optical absorption of the molecule, the Raman G-band signal exhibits a weak but significant up or downshift depending on the nanotube diameters. This behavior is consistent with a permanent electron transfer to the nanotube in the framework of the renormalization process [1]. In addition, close to the molecule resonance, the magnitude of the G-band shift is enhanced for small diameter tubes, evidencing a photo-induced electron transfer. Finally, the Breit-Wigner-Fano lineshape (characteristic of electron-phonon coupling) of the Raman G-band can be strongly reduced for defective metallic nanotubes. After molecule functionalization, this peculiar profile is recovered, suggesting a back donation of electrons to the nanotube. Photoluminescence properties of semiconducting nanotubes are also significantly modified by chromophore confinement. The nanotube emission intensity is amplified after encapsulation. This exaltation depends on the nanotube diameter, and can be related to diameters exactly fitting the molecule size. The origin of the photoluminescence enhancement will be discussed.

[1] Tsang, J. C.; Freitag, M.; Perebeinos, V.; Liu, J.; Avouris, P. *Nanotechnol.* 2007, 2, 725

S2-4: Biometrology Enabled by Carbon Nanotube Optical Bandgap Modulation

Heller, Daniel (Memorial Sloan Kettering Cancer Center, New York, USA)

Single-walled carbon nanotubes have properties that make them ideally suited for detection of biologically important analytes. Carbon nanotubes exhibit bandgap photoluminescence which does not photobleach or blink, and emission can be modulated by changes in the immediate environment. Tissue transparent emission, biocompatibility, and versatile modes of optical response make SWCNTs uniquely valuable optical biosensors. Using these properties, we have rationally designed SWCNT-based sensors for enhanced quantification of biomarkers in biofluids for diagnostic applications and for the study of fundamental biological processes. We monitored shifts in nanotube emission wavelength, caused by changes in the optical bandgap in response to solvent dielectric and electrostatic charge. The responses can be spatially mapped in live cells and tissues, and measured in real-time, facilitating unprecedented bioanalytical studies.

S2-5: Carbon based materials - a health perspective

Wick, Peter (Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, CHE)

Carbon based materials (CBM) have attracted enormous attention due to their outstanding properties enabling innovative technological applications across nearly all areas of development. However, as for all new technologies, a safe and sustainable production as well as use of GBM is a prerequisite for economical and societal success. Due to its emerging nature the potential risks of CBM released into the environment during production, use or disposal, for human and environment have to be investigated properly. Carbon nanotubes (CNTs) are being manufactured at a range of a few to hundred tons per year and mostly used to reinforce polymers. Graphene and graphene related materials (GRM) the most prominent 2D materials, have become a lodestar for research and development, indicated by the highly increasing number of publications and patents. Therefore it is likely that human get exposed via the skin, the blood circulation or the gastrointestinal tract. Nonetheless, inhalation is widely accepted as the primary route of entry for nanomaterials, especially when considering occupational exposure. Therefore the aim of this paper is to i) summarize the current knowledge about CNT toxicity, the influence of their functionalization on cellular uptake and cellular response as well as their biodegradation. ii) assess the current knowledge of GRM toxicity, the current challenges to correlate the physico-chemical properties of GRM and their biological responses and finally iii) explore and qualify the knowledge about the release of CBM from nanocomposites after mechanical treatment and assess the potential hazard of the released materials.

S2-6: Compared ecotoxicity of carbon-based nanoparticles on *Xenopus laevis* tadpole

Lagier, Laura (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA); MOUCHET, Florence (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA); CADARSI, Stéphanie (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA); MOTTIER, Antoine (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA); FLAHAUT, Emmanuel (Institut Carnot CIRIMAT, UPS-INP-CNRS, Toulouse, FRA); SARRIEU, Cyril (Institut Carnot CIRIMAT, UPS-

INP-CNRS, Toulouse, FRA); ARNAULT, Jean-Charles (3CEA, Diamond Sensors Laboratory, F-91191 Gif sur Yvette, Gif sur Yvette, FRA); GIRARD, Hugues (CEA, Diamond Sensors Laboratory, F-91191 Gif sur Yvette, Gif sur Yvette, FRA); MENARD-MOYON, Cécilia (CNRS, IBMC, UPR 3572, F-67084 Strasbourg, Strasbourg, FRA); JANOWSKA, Izabela (ICPEES, CNRS-Université de Strasbourg, UMR 7515, Strasbourg, FRA); BIANCO, Alberto (CNRS, IBMC, UPR 3572, F-67084 Strasbourg, Strasbourg, FRA); VAZQUEZ, Ester (UCLM, MSOC Nanochemistry Group, DOC, IRICA, Ciudad Real, ESP); PINELLI, Eric (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA); GAUTHIER, Laury (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA)

The production of carbon-based nanoparticles (CNPs) is rapidly increasing worldwide. Their outstanding properties lead to their use in many application fields, but may also make them very reactive with their environment. Currently, hazard associated with these emerging contaminants are still not well evaluated. Anticipating environmental risks is crucial, especially concerning the aquatic environment, which is a major pollution receptacle. The present work aims to assess and to compare the ecotoxicity of well characterized raw CNPs: double and multi-walled carbon nanotubes (DWCNTs, MWCNTs), few-layer graphenes (FLG₁, FLG₂), nanodiamond (ND) and carbon black (CB). Functionalized CNPs such as graphene oxide (GO) and reduced GO (rGO) were also tested. Their toxicity were investigated using the ISO 21427-1 standardized procedure on amphibian larvae (*Xenopus laevis*). The exposure concentrations ranged from 0.05 to 50 mg.L⁻¹. Various endpoints were studied: acute toxicity (mortality), chronic toxicity (growth inhibition), and genotoxicity (induction of micronucleated erythrocytes). Neither mortality nor genotoxicity were observed whatever the raw CNP exposure (type and concentration). However, significant growth inhibition was observed from 0.1 mg.L⁻¹ of CB, 1 mg.L⁻¹ of ND, 10 mg.L⁻¹ of DWCNT and FLG₂, and at 50 mg.L⁻¹ of MWCNT, FLG₁ and GO. Only GO induced a significant genotoxicity at 0.1 mg.L⁻¹, whereas no genotoxic effect was recorded when GO is reduced. Macro-observations suggested that the chronic toxicity in larvae exposed to the highest concentrations of CNPs could be limited to physical effects such as gill clogging and intestinal obstruction, which could cause respiratory deficiency and/or abrasive effects and/or nutrients deprivation. The observed genotoxicity may be in relation with the surface chemistry of GO. However larvae were not significantly impacted at high concentration of GO, which may also be related to a decreased mitotic index.

S2-7: Flexible carbon nanotube interdigitated electrode for electrochemical biosensors

Ushiyama, Takuya (Graduate School of Engineering, Nagoya University, Nagoya, JPN); X Nguyen, Viet (Graduate School of Engineering, Nagoya University, Nagoya, JPN); Kishimoto, Shigeru (Graduate School of Engineering, Nagoya University, Nagoya, JPN); Ohno, Yutaka (Institute of Materials and Systems for Sustainability, Graduate School of Engineering, Nagoya University, Nagoya, JPN)

Electrochemical biosensors have attracted much attention because of their potential to realize small-sized point-of-care testing devices. Single-walled carbon nanotube (CNT) thin film is promising material for electrochemical sensors because of its

excellent electrochemical properties, i.e., wide potential window, rapid electron transfer kinetics, anti-fouling property and so on. In this work, we have utilized the redox cycle to enhance the sensitivity with an interdigitated electrode (IDE) composed of a CNT thin film. The detection of dopamine (DA) has also been demonstrated with the CNT-IDE. For the electrochemical application of CNT thin films, it is important to realize a CNT thin film with clean surface. Therefore, we employed the dry transfer process to form a CNT thin film [1], in which CNTs were grown by the floating-catalyst CVD, collected on the membrane filter, and then transferred on a plastic film without contaminations. We also protected the CNT film with SiO₂ from contamination in the sensor fabrication process. The fabricated CNT-IDEs were characterized by four-electrode cyclic voltammetry of K₄[Fe(CN)₆]. The signal current was 14 times higher than conventional planar electrode, showing collection efficiency of higher than 90 %. We also performed the detection of DA, an important neurotransmitter, with the CNT-IDE. The CNT-IDE exhibited good linearity in the detection of DA from 10 nM to 1 μM, covering the DA concentration in blood. Selective detection of DA in ascorbic acid (AA), known as vitamin C, was also demonstrated. The limit of detection of DA was 10 nM in 0.1-mM AA.

[1] A. Kaskela *et al.*, Nano Lett., **10**, 4349 (2010)

S2-8: Red Blood Cell Hemolysis under Mechanical Stress as a Physiologically-Relevant Tool for Testing of Nanotubes Toxicity.

Barshtein, Gregory (The Hebrew University-Medical School, Jerusalem, ISR); Shvartsman, Leonid D (The Hebrew University, Jerusalem, ISR); Yedgar, Saul (The Hebrew University-Medical School, Jerusalem, ISR)

Engineered nanomaterials (NM) have various applications in biomedical fields, mainly for diagnostics and drug delivery. Independent of their target, source and method of administration, NM eventually enter the blood stream and interact with red blood cells (RBC), the major blood constituent. This may impair RBCs functionality, and cause their hemolysis. Hemolysis may occur if the integrity of RBCs membrane is broken and the hemoglobin is released. Therefore, the hemolytic activity of NM can be used for the assessment of NM toxicity. Although NM hemolytic activity has been in various studies, comparing their results is difficult due to the variability in the protocols used for NM characterization and the hemolysis tests. Notably, in all previous studies, the interaction between NM and RBC was examined under stasis (no flow), which does not reflect the physiological condition. In the presented study, we examined the hemolytic activity of *carboxylic acid functionalized multi-walled carbon nanotubes (MWCNT)*, under mechanical stress, resembling the shear stress applied to RBC in the blood circulation. It was found that the hemolytic activity of MWCTN (5 - 50 μg/ml) was insignificant under stasis, but clearly amplified with increased mechanical stress. These findings demonstrate for the first time that effect of carbon nanotubes on RBC should be tested under stress conditions, and present a novel, physiologically-relevant methodology for testing NM toxicity.

S2-9: The effect of carbon nanohorns on human monocyte and mesenchymal stem cells

Hirata, Eri (Department of Oral Functional Prosthodontics, Graduate School of Dental Medicine, Hokkaido University, Sapporo, JPN); Miyako, Eijiro (Department of Materials and Chemistry, Nanomaterial Research Institute (NMRI), National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN); Yudasaka, Masako (Nanotube Research Center, National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN); Bianco, Alberto (CNRS, Institut de Biologie Moléculaire et Cellulaire, Laboratoire d'Immunopathologie et Chimie Thérapeutique, Strasbourg, FRA); Yokoyama, Atsuro (Department of Oral Functional Prosthodontics, Graduate School of Dental Medicine, Hokkaido University, Sapporo, JPN)

Carbon nanohorns (CNHs) consist of a rolled graphene structure with cone-shaped tips, which are currently developed for biological applications. Previously, we have reported that CNHs promote rat calvarial bone formation. In order to find the mechanism of the bone formation, we focused our attention on the effect of the human monocyte derived macrophages (hMDM) loaded with CNHs on osteoblast differentiation. At first, in order to explore cell response to CNHs, microarray analysis was carried out after culturing hMDMs with CNHs. Microarray analysis indicates that chemokine-related genes, including CCL3, CCL4, and CXCL12, were expressed significantly higher in hMDMs treated with CNHs than without CNHs. GO analysis suggests that these upregulated genes regulate lymphocyte migration. After coculturing hMDM with human mesenchymal stem cells (hMSCs) in the presence of CNHs, CNHs were observed in the lysosomes of macrophages more than in mesenchymal stem cells and alkaline phosphatase activity dramatically increased. At the same time the amount of Oncostatin M (OSM), which is reported that induce osteoblast differentiation and matrix mineralization, was much more in the supernatant cultured with CNHs than those without CNHs. These results demonstrate that the macrophages engulfed CNHs thus accelerating the differentiation of mesenchymal stem cells into the osteoblasts via OSM. This study demonstrates one of the possible mechanisms for bone formation with CNHs and CNHs could be applied for bone regeneration.

S2-10: 2D nanomaterials in Biomedicine: Graphene and Beyond

Liu, Zhuang (Soochow University, Suzhou, CHN)

Two-dimensional (2D) nanomaterials, such as graphene, have attracted tremendous interests in many different fields including biomedicine in recent years. With every atom exposed on its surface, single-layered graphene shows ultra-high surface area available for efficient molecular loading and bioconjugation, and has been widely explored as novel nano-carriers for drug and gene delivery. Utilizing the intrinsic near-infrared (NIR) optical absorbance, in vivo graphene-based photothermal therapy has been realized, achieving excellent anti-tumor therapeutic efficacy in animal experiments. A variety of inorganic nanoparticles can be grown on the surface of nano-graphene, obtaining functional graphene-based nanocomposites with interesting optical and magnetic properties useful for multi-modal imaging and imaging-guided cancer therapy. Moreover, significant efforts have also been devoted

to study the behaviors and toxicology of functionalized nano-graphene in animals. It has been uncovered that both surface chemistry and sizes play key roles in controlling the biodistribution, excretion, and toxicity of nano-graphene. In this talk, I will summarize our research in the exploration of graphene for biomedical applications, and introduce our recent studies for other types of 2D nanomaterials beyond graphene.

S2-11: Flexible carbon nanotube interdigitated electrode for electrochemical biosensors

Ushiyama, Takuya (Graduate School of Engineering, Nagoya University, Nagoya, JPN); X Nguyen, Viet (Graduate School of Engineering, Nagoya University, Nagoya, JPN); Kishimoto, Shigeru (Graduate School of Engineering, Nagoya University, Nagoya, JPN); Ohno, Yutaka (Institute of Materials and Systems for Sustainability, Graduate School of Engineering, Nagoya University, Nagoya, JPN)

Electrochemical biosensors have attracted much attention because of their potential to realize small-sized point-of-care testing devices. Single-walled carbon nanotube (CNT) thin film is promising material for electrochemical sensors because of its excellent electrochemical properties, i.e., wide potential window, rapid electron transfer kinetics, anti-fouling property and so on. In this work, we have utilized the redox cycle to enhance the sensitivity with an interdigitated electrode (IDE) composed of a CNT thin film. The detection of dopamine (DA) has also been demonstrated with the CNT-IDE. For the electrochemical application of CNT thin films, it is important to realize a CNT thin film with clean surface. Therefore, we employed the dry transfer process to form a CNT thin film [1], in which CNTs were grown by the floating-catalyst CVD, collected on the membrane filter, and then transferred on a plastic film without contaminations. We also protected the CNT film with SiO₂ from contamination in the sensor fabrication process. The fabricated CNT-IDEs were characterized by four-electrode cyclic voltammetry of K₄[Fe(CN)₆]. The signal current was 14 times higher than conventional planar electrode, showing collection efficiency of higher than 90 %. We also performed the detection of DA, an important neurotransmitter, with the CNT-IDE. The CNT-IDE exhibited good linearity in the detection of DA from 10 nM to 1 μM, covering the DA concentration in blood. Selective detection of DA in ascorbic acid (AA), known as vitamin C, was also demonstrated. The limit of detection of DA was 10 nM in 0.1-mM AA. [1] A. Kaskela *et al.*, *Nano Lett.*, **10**, 4349 (2010)

S2-12: Linking nanomechanical mechanisms to carbon nanotube-induced toxicity

von dem Bussche, Annette, Wenpeng Zhu, Xin Yi, Yang Qiu, Zhongying Wang, Paula Weston, Robert H. Hurt, Huajian Gao & Agnes B. Kane, Brown University, Providence, Rhode Island, USA.

The toxicity of carbon nanotubes has been widely studied, and due to variations in nanotube size, shape, dimensions, surface chemistry and impurities, investigations have shown different toxicity outcomes using various target cells in vitro. We hypothesize that nanomechanical interactions between one-dimensional

nanomaterials and target cells are also important determinants of their toxicity. One-dimensional or high aspect ratio nanomaterials can mechanically damage biological structures including the plasma membrane, the cytoskeleton, and lysosomes. Following cell uptake, stiff or rigid one-dimensional carbon nanotubes may cause stress or deformation when packaged into soft spherical vesicles or lysosomes. We determine the precise material parameters that mechanically activate this toxicity pathway through coupled simulations and experimental studies using a panel of carbon nanomaterials with systematic variations in size, shape, and stiffness. Using biochemical assays and a variety of imaging methods in combination with quantitative single-cell confocal fluorescence imaging, we demonstrated that only long and stiff MWCNTs cause lysosomal permeabilization and release of cathepsin B, leading to activation of caspases and cell death. This study will contribute to a better understanding of nanomechanical mechanisms responsible for the toxicity of one-dimensional, high aspect ratio nanomaterials as a key to their safe design.

This work was supported by NSF (CMMI-1028530, CBET-1132446 and CBET-1344097), Superfund Research Program NIEHS (Grant P42 ES013660), and NICS (MS090046).

4th Carbon Nanotube Thin Film Electronics and Applications Satellite	
9:00-9:30	Invited Talk: Kenji Hata
	<i>Fabrication of CNT films and the rational CNT applications made from them. (S3-12)</i>
9:30-10:00	Invited Talk: Suguru Noda
	<i>Production and functionalization of carbon nanotubes for electrically conductive thin films and electrochemically capacitive thick films (S3-4)</i>
10:00-10:10	Contributed Talk: Keizo Iseki
	<i>Carbon Nanotube Electrodes - enhanced Redox Flow Batteries Performance (S3-1)</i>
10:10-10:20	Contributed Talk: Fumiaki Tanaka
	<i>High performance micro-supercapacitors with thick carbon nanotube film electrodes on a thin polymer substrate (S3-13)</i>
10:20-10:30	Contributed Talk: Tomohiro Yasunishi
	<i>The voltage generation by movement of electrolyte solution on carbon nanotube thin film (S3-20)</i>
10:30-10:50	Coffee Break & Poster Session
10:50-11:00	Contributed Talk: Hua An
	<i>Chirality selective synthesis of single-walled carbon nanotubes with sputtered Co-W as catalyst (S3-22)</i>
11:00-11:10	Contributed Talk: Patrik Laiho
	<i>Direct and controlled deposition of aerosol synthesized single-walled carbon nanotubes for electronics and photonics (S3-9)</i>
11:10-11:20	Contributed Talk: Kentaro Yamada
	<i>Fabrication of low-resistivity CNT-TCFs by spray deposition (S3-2)</i>
11:20-11:30	Contributed Talk: Kimmo Mustonen
	<i>The ultimate performance of single-walled carbon nanotubes as transparent conductors? (S3-19)</i>
11:30-11:40	Contributed Talk: Aqeel Hussain
	<i>Dry manufacturing of SWNT transparent conducting films with FC-CVD from ethylene in nitrogen atmosphere (S3-10)</i>
11:40-11:50	Contributed Talk: Keigo Otsuka
	<i>Voltage-driven physical gap extension of single-walled carbon nanotubes after electrical breakdown (S3-21)</i>
11:50-12:00	Contributed Talk: Yingjun Yang
	<i>High performance CMOS FETs based on carbon nanotube film and their applications for medium scale integrated</i>

	<i>circuits (S3-3)</i>
12:00-12:10	Contributed Talk: Jun Hirotani
	<i>Transparent and stretchable all-carbon nanotube thin-film transistors for wearable electronics (S3-6)</i>
12:10-12:20	Contributed Talk: Stefan P. Schießl
	<i>Influence of self-assembled monolayer dielectrics on network density and device performance of SWNT transistors (S3-14)</i>
12:20-13:30	Lunch
13:30-13:40	Contributed Talk: Arko Graf
	<i>Strong light-matter coupling of single-walled carbon nanotubes in microcavities (S3-17)</i>
13:40-14:10	Invited Talk: Jana Zaumseil
	<i>Photonic, electronic and optoelectronic applications of polymer-sorted semiconducting carbon nanotubes (S3-15)</i>
14:10-14:20	Contributed Talk: Luis A. Panes Ruiz
	<i>Efficient ammonia sensors based on single walled carbon nanotubes (S3-11)</i>
14:20-14:30	Contributed Talk: Lei Shi
	<i>Confined linear carbon chains: Synthesis and properties (S3-23)</i>
14:30-14:40	Contributed Talk: Salome Forel
	<i>Synthesis optimisation of SWNTs for nanoelectronic device's (S3-18)</i>
14:40-16:00	Poster Session
16:00-16:30	Invited Talk: Dongming Sun
	<i>Scale-up fabrication of single wall carbon nanotube thin film and its application in flexible thin-film transistors (S3-16)</i>
16:30-17:00	Invited Talk: Jacques Lefebvre
	<i>Thin Film Transistors from Polymer Sorted SWCNTs (S3-5)</i>
17:00	Closing the Satellite

CNTFA16: 4th Carbon Nanotube Thin Film Electronics and Applications Satellite

S3-1: Carbon Nanotube Electrodes-enhanced Redox Flow Batteries Performance.

Iseki, Keizo (SHOWA DENKO K.K., Chiba-shi, JPN); Irwansyah (SHOWA DENKO K.K., Chiba-shi, JPN); Oriji, Gaku (SHOWA DENKO K.K., Chiba-shi, JPN); Ichikawa, Masatoshi (SHOWA DENKO K.K., Chiba-shi, JPN); Hanawa, Kenzo (SHOWA DENKO K.K., Chiba-shi, JPN)

Vanadium Redox Flow Battery (VRFB) is a major candidate for stationary battery as storage of renewable energy and emergency power supply. In this type of flow battery, carbon felt and carbon paper made of carbon fiber are generally used as electrode. However, due to unexpected oxidation, the durability of those electrodes is facing some challenge, especially if the battery is expected for running more than 10 years. Carbon nanotubes (CNTs) are known as potential material for redox electrode due to its large specific surface area and chemical stability. In spite of high reactivity of CNT itself¹, the powder nature of CNT causes it difficult to fabricate into a sheet-like electrode for VRFB. Consequently the performance of CNT as sheet-like electrode for VRFB was not verified. In our work, we developed a new low cost and high performance of VRFB using sheet-like carbon nanotube as electrode. Sheet-like CNT electrode was fabricated by mixing two different types of multi-walled CNT. As observed by STEM, the entanglement of two different types of CNT may contribute to the improved formability. The high reactivity of sheet-like CNT electrode toward vanadium ion in aqueous solution was verified by cyclic voltammetry. Redox current peaks which correspond to redox reaction not only between V(II) and V(III), and between V(IV) and V(V) but also between V(III) and V(IV) were observed. This indicates CNT electrode can be used for VRFB. CV result suggests that high reactivity of the graphene basal surface, which constitutes the majority of the surface of CNTs. To make the most of CNT electrode, we invented new type of flow design and with this design, excellent charge and discharge performance were obtained. Small amount of CNT (<100 g/m²) enables charge and discharge at higher current densities than conventional carbon paper electrodes. This means CNT electrode has lower cost and higher performance than existing electrodes.

[1] Ulrich Stimming *et al.*, *Carbon*, **63** (2013), 228-239

S3-2: Fabrication of low-resistivity CNT-TCFs by spray deposition

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Carbon nanotube transparent conductive films (CNT-TCFs) are potential candidates as Indium-based TCO films for the applications of transparent electrodes. However, it has been difficult to prepare CNT-TCFs with low cost deposition when the films are deposited on glass substrate. Therefore, in order to obtain the high-quality CNT-TCFs with low cost deposition, substrate materials are being replaced by a flexible material such as PET. For utilizing unique electric, mechanical and structural properties of CNTs, it is necessary to disperse them into solvents. Taking these factors into consideration, a wet type roll to roll process is thought to be best for fabrication of CNT-TCFs. In this work, we succeeded in fabrication of low-resistivity CNT-TCFs on a PET substrate by our spray deposition system. To fabricate low-resistivity CNT-TCFs, surfactants added in CNT-TCFs fabrication process should be removed because they remain on the surface of the CNT layer, causing conductivity degradation. We found that surfactants can be removed efficiently by flushing the substrate surface with water at every CNT deposition step. The lowest sheet resistance of CNT-TCFs was 480 ohm/□ on PET substrate. Transmittances in visible region for these CNT-TCFs were more than 77%. Thus, we show that the whole process from the fabrication of low-resistivity CNT-TCFs to forming pattern for touch sensors can be realized by a roll to roll photolithography process.

S3-3: High performance CMOS FETs based on carbon nanotube film and their applications for medium scale integrated circuits

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Carbon nanotube (CNT) thin films prepared through CNT solution with high semiconducting purity is the material suitable to construct field-effect transistors (FETs) and integrated circuits (ICs) in wafer scale. As we all known, complementary metal-oxide-semiconductor (CMOS) is the mainstream circuit style for modern ICs owing to the lower static power dissipation and high noise margin. However it is difficult to realize high performance CMOS FETs with high yield and stability on CNT networks, which hinders the development of high performance and lager scale CNT ICs. In this work, we developed a doping free process to fabricate top-gated CMOS FETs based on CNT network film from CNT solution, and the n-type FETs were realized through using the low work function metal scandium as source/drain contacts. With a well-developed self-aligned gate structure, the CMOS FETs with gate length of 5 μm present high and symmetric performance, including on-current, transconductance, and subthreshold slope swing, as well as high yield up to 100%. Benefitted from high performance of CNT CMOS FETs, various logic and functional gates such as NOT, NAND, NOR, AND, OR, XOR, XNOR, MUX2_1, D-latch have been fabricated with rail-to-rail output. Particularly the fabricated CMOS inverter presents symmetric input/output behavior and large noise margin, and can be

powered by a low supply voltage scaled down to 0.1V. Taking full advantages of high yield and stability of CNT CMOS FETs, medium scale ICs such as a four-bit serial carry adder consisting of 132 FETs, have been successfully demonstrated with yield of 100%. All the results indicated that CNT CMOS FETs are ready for constructing large-scale or even very-large scale ICs in batch

S3-4: Production and functionalization of carbon nanotubes for electrically conductive thin films and electrochemically capacitive thick films

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Carbon nanotube (CNT) network is attractive for film applications owing to its easy fabrication, fair conductivity, lightness, flexibility, high specific surface area, and stability. Transparent conductive films (TCFs) are attractive; 1 m² TCFs use only 5–10 mg CNTs and cost effective. But such small amount of CNTs need to support electrical conduction. Among various methods, aqueous solution-based dispersion-printing is popular due to its mild condition. Excellent performances have been reported, however, often by using supernatant of mildly dispersed and centrifuged CNTs while wasting remaining sediment. Strong dispersion enables full dispersion but yields short and damaged CNTs. We proposed repetitive dispersion-centrifugation process, and overcame the quality-quantity trade-off. We sonicated CNTs for 3 min, centrifuged, used the supernatant for films while added surfactant solution to and re-sonicated the sediment. 13 cycles converted CNTs at >90% into printed lines of ~2000 S/cm without doping, and TCFs with 80% transmittance and 50 Ω/sq resistance were realized with HNO₃ doping [1]. Continuous dispersion-extraction process will also be presented. Battery/capacitor electrodes are also attractive in which carbon black and carbon nanofibers have been used as conductive fillers. Small-diameter CNTs show unique self-supporting nature, and we are trying to replace heavy 2D metal foils with light-weight 3D CNT sponges for current collectors. We use long CNTs by fluidized bed [2] for CNT sponges. Electrodes of activated carbon particles captured in 10 wt% few-wall CNTs realized capacity x3 of pure single-wall CNTs [3], and worked with metal contact on only their edge [4]. Electrodeposition of MnO₂ nanoparticles in CNT papers realized thick pseudocapacitive electrodes. 1 wt% CNTs realized self-supporting LiCoO₂ cathodes and graphite anodes, which minimized the use of metal foils in lithium ion batteries. CNT-sponge based S cathodes and Si anodes will also be presented.

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S3-5: Thin Film Transistors from Polymer Sorted SWCNTs

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The practical use of SWCNTs as the semiconductor channel in printable electronics applications relies on two important efforts: 1. Formulation and printing of an ink highly enriched in semiconductor SWCNTs; 2. Identification of transistor

architecture and corresponding choice of dielectric materials that produces stable device performance. In this contribution, activities within our Printable Electronics program that address those challenges will be presented. Our ink formulation is primarily based on the selective affinity/solubility of sc-SWCNTs for conjugated polymers in organic solvents. Our process is optimized to efficiently extract larger diameter carbon nanotubes (1.3 nm) produced in a commercial scale plasma system.[1] Absorption and Raman spectroscopy show ultra-low metal-SWCNTs content while bright luminescence is observed with (10,9) chirality being dominant in PLE maps.[2] Transistor devices fabricated from soaking have high current carrying capacity of $\approx \mu\text{A}/\mu\text{m}$ channel width, and calculated field effect mobility in excess of $35 \text{ cm}^2/\text{Vs}$ and $\text{On/Off} > 10^5$. [3] Printing of sc-SWCNT wrapped with conjugated polymer is achieved using two methods: commercial inkjet and custom-designed aerosol. In both cases, dispersions are used without additives and transistors with sub-150 μm channel length have performance similar to soaking. With inkjet, a fully printed transistor is demonstrated with mobility of $1 \text{ cm}^2/\text{Vs}$. [4] With its unique attributes, aerosol provides a solution to deposit SWCNTs on the most difficult surfaces, including hydrophobic polymers such as Teflon-AF. Bottom gated transistors are shown to have little hysteresis and excellent temporal stability, even under bias stress. [5] Opportunities for applications using our SWCNT-based materials package together with our printing capabilities will be presented.

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S3-6: Transparent and stretchable all-carbon nanotube thin-film transistors for wearable electronics

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Flexible and stretchable electronics have been intensively explored for wearable and bioimplantable applications such as electronic-skins and healthcare/medical devices. Carbon nanotube (CNT) thin-films are a promising candidate for their applications due to their excellent carrier mobility, mechanical flexibility, transparency and chemical stability. In addition, CNT thin-film can be used both as a metallic conductor and as a channel material for high-performance transistors [1], which enables to fabricate the high-performance and transparent all-carbon devices providing a possibility of realizing wearable devices without feeling its existence. In this work, we have fabricated stretchable and transparent all-CNT transistors on poly(dimethylsiloxane) (PDMS) substrates. The uniaxial stretching test have also been performed. The device fabrication was carried out on a Si substrate, and subsequently the devices were transferred on a PDMS substrate. The CNT electrodes

were formed by the dry transfer process based on the floating-catalyst CVD [2] and subsequent photolithography process. Semiconducting CNTs purified by the gel chromatography [3] were used as the channel material. One-dimensional tensile strain test showed a small degradation in drain current as 8 % under the tensile strain of 20%. We also confirmed that the device worked even for 40% tensile strain, and the drain current returned to the initial value when the strain was released.

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S3-7: Chirality selective synthesis of single-walled carbon nanotubes with sputtered Co-W as catalyst

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The application of single-walled carbon nanotubes (SWNTs) in nanodevices is limited by impurities and mixed chiralities of SWNT assemblies. Great efforts have been made in the purification and separation of SWNT mixtures. However, direct synthesis of SWNTs with a single chirality is still challenging. CoW clusters were reported to grow a single chirality SWNT (12, 6), with over 90% enrichment and a zigzag SWNT (16, 0), with near 80%, by controlling the catalyst structure and growth conditions via a high-temperature reduction and growth [1, 2].

Recently, we succeeded in selectively growing (12, 6) SWNTs with sputtered CoW catalyst by low pressure alcohol catalytic chemical vapor deposition at low temperature [3]. The abundance of (12, 6) is over 50% according to the statistical Raman mapping analysis and optical absorption spectrum of the as-grown SWNTs. Parametric study of the CoW catalyst system demonstrates that the reduction temperature before growth is critical for the selectivity and the intermediate structure, Co₆W₆C, is identified by the electron diffraction. Most of tungsten atoms are found to be removed after 5 min growth with only cobalt remained on the substrate, which discloses the complicated structure changes before and after growth. More details will be discussed on investigation of the morphology and structure of catalysts by transmission electron microscopy and electron diffraction.

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S3-8: Confined linear carbon chains: Synthesis and properties

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The extreme instability and strong chemical activity of carbyne, the infinite sp^1 hybridized carbon chain, are responsible for its low possibility to survive at ambient conditions. We successfully synthesized extremely long linear carbon chains (LLCCs) inside thin double walled carbon nanotubes as nanoreactors and protectors [1]. Their existence, structure, lengths and yield have been proved by Raman, HRTEM, STEM and XRD. The results show that the single-triple bonded LLCCs including thousands of carbon atoms have at least six new Raman peaks, some of which are even stronger than the G-band. The optimum growth conditions, for example, diameter of the host tubes, annealing temperatures and time were carefully studied. The interaction and charge transfer between the LLCCs and their host nanotubes were explored using resonance Raman, low-temperature Raman and DFT calculations. Furthermore, the band gap of the LLCCs was examined by resonance Raman spectroscopy. The results suggest that the band gap of LLCCs in the range of 1.8 - 2.3 eV is inversely proportional to their lengths, which is also perfectly consistent with our DFT calculations.

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[3] Shi et al. Band gap of long linear carbon chains. In preparation.

S3-9: Direct and controlled deposition of aerosol synthesized single-walled carbon nanotubes for electronics and photonics

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Thermophoresis, or the force exerted on aerosols by a temperature gradient, provides a continuous, dry and clean way of depositing nanosized aerosols such as SWCNTs grown using the floating catalyst CVD (FC-CVD) process. Using thermophoretic precipitators we can deposit clean, as-synthesized SWCNTs on centimeter-sized substrates with controllable densities, ranging from individual separated nanotubes to thin films. Based on loss measurements by aerosol methods, high deposition efficiencies ranging from 50% to 90% can be obtained and predicted by simple equations of motion.[1] By depositing sub-monolayers of SWCNTs and investigating their morphology using atomic force microscopy, we have established that gas-phase bundling in the FC-CVD process can be described by aerosol agglomeration caused by Brownian motion[2,3]. We have also fabricated network channel TFTs with high

charge carrier mobilities and ION/IOFF ratios comparable to previously published devices fabricated using filter dissolution[1,4]. We have also carried out photoluminescence spectroscopy of FC-CVD SWCNTs for the first time by depositing air-suspended nanotubes on trenches, using a method previously reported for SWCNTs grown using surface CVD[5]. Finally, we have fabricated aligned arrays of SWCNTs, applicable to nanoscale CNTFETs, by introducing a dielectrophoretic force using planar electrodes.[6]

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S3-10: Dry manufacturing of SWNT transparent conducting films with FC-CVD from ethylene in nitrogen atmosphere

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The single-walled carbon nanotubes (SWCNT) thin film stands as a strong candidate for replacement of indium-tin oxide (ITO) in transparent electrodes. The length of nanotubes is critical to achieve high conductivity SWCNTs transparent conducting films (TCF) due to smaller number of resistive junctions with the longer tubes (1). The synthesis process of using carbon monoxide (CO) as carbon source is limited to produce longer SWCNTs owing to its thermodynamically limited i.e. rather low synthesis temperature. Moreover, the CO process has usually low yield, and CO is expensive and challenging to operate safely. In this contribution, we demonstrate high yield synthesis of SWCNTs in floating catalyst CVD (FC-CVD) using C₂H₄ hydrocarbon as the carbon source and nitrogen with small amount of hydrogen as the carrier gas. The nitrogen environment makes the SWCNTs growth process safer and also largely cuts the running cost. Our results show that the C₂H₄-N₂-H₂ FC-CVD reactor operated at 1050 °C and using ferrocene vapor based Fe catalyst particles produced relatively long bundles with an average length up to 16 μm, while the similar reactor operated at CO produced tubes with just 4 μm average length. This ethylene process produced long SWCNTs while keeping mean diameter below 1.5 nm. With such long SWCNTs, highly conductive transparent films were achieved, with the sheet resistance of 200 ohm/sq. at 90 % transmittance at a wavelength of 550nm without doping. The doping the film with gold chloride (AuCl₃) in acetonitrile solution further reduced the sheet resistance down to 60 ohm/sq. at 90% transmittance at 550 nm.

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Y., Zhu, Z., Jiang, H., Brown, D.P., Zakhidov, A. and Kauppinen, E.I., NanoLetters 10, 4349 (2010)

S3-11: Efficient ammonia sensors based on single walled carbon nanotubes

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Carbon nanotubes have emerged as a promising alternative for highly efficient gas sensing technologies due to their remarkable properties like high surface to volume ratio and the possibility of doping or functionalization according to a specific application. In this work, the response of gas sensing devices based on networks of single walled semiconducting, pristine (unsorted), boron doped and nitrogen doped carbon nanotubes to small concentrations of ammonia at room temperature was investigated. Moreover, the recovery properties after 3 weeks in controlled conditions of temperature (22°C) and humidity (30%) were also studied. The sensors were fabricated using UV-lithography process and the nanotubes were deposited using a drop casting approach followed by electrical and scanning electron microscopy characterization. Then, the sensors were exposed to 1.5, 2.5, 5, 10 and 20 ppm of NH₃ in a chemiresistor configuration, and the change of current at a fixed voltage as the reaction to the gas exposure was measured. Sensor characterization demonstrated that the distribution of deposited nanomaterial between electrodes and the sensing properties of the sensor are closely related. Sensors based on semiconducting CNTs exhibited the highest sensing responses to all ammonia concentrations compared to other nanotubes. These sensors are able to reliably detect 1.5 ppm of ammonia at room temperature within 100 seconds of exposure.

S3-12: Fabrication of CNT films and the rational CNT applications made from them.

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The CNT film is the crucial material for many applications. In this talk, I would overview our efforts, over the last decade, to fabricate CNT films, pattern them into functional components, and to develop rational CNT devices. Our initial efforts used and was focused on thin self-standing aligned CNT films directly synthesized by CVD and transferred to the device substrate. These films enabled to realize many devices with very high performances such as strain-sensors, bio-energy devices, CNT-Cu wires with high ampacity and super-capacitors. While these works brought insights into promising directions for CNT devices, the use of thin aligned CNT films made by CVD limited the development of real commercial products. Therefore, we have from CNT dispersions. Currently, we have succeeded in fabricating CNT dispersions without surfactants that can be coated into CNT films and patterned subsequently for CNT devices. This approach is scalable and would enable mass production of the aforementioned CNT devices.

S3-13: High performance micro-supercapacitors with thick carbon nanotube film electrodes on a thin polymer substrate

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Micro-supercapacitors have attracted increasing attention due to their high power density, durability and safety compared to other energy devices. Compared to conventional supercapacitors, miniaturization of the structure and fabricating the components on a substrate (e.g., Si) result in higher power density and quick frequency response owing to reducing the ion traveling length. Recently, our group succeeded in developing high-performance single-walled carbon nanotube (SWCNT) micro-supercapacitors to have high energy and power densities similar to commercially available aluminum electrolytic capacitors, reducing the size to 1,000 times smaller than them at the same time (Adv. Energy Mater.5, 1500741 (2015)).

However, the drawback of micro-supercapacitors is their relatively small energy capacity because their small volume of electrodes cannot store much amount of ions. For industrialization, thicker electrodes are desirable to increase the energy capacity, resulting in the increased areal energy density. Furthermore, if the components can be fabricated on a thinner substrate, the volumetric energy density for an entire device can be dramatically improved. Also, such thin film micro-supercapacitors are promising candidates as energy sources for flexible/wearable electronics.

Here, we developed a fabrication process of micro-supercapacitors possessing thick film of SWCNT electrodes on a very thin polymer substrate ($< 2 \mu\text{m}$), where electrodes occupied more than 75% of space in the entire device. As a result, compared to conventional CNT/graphene micro-supercapacitors on a Si substrate ($\sim 0.6 \text{ mm}$), energy and power densities can be increased more than 75 fold when considering all device components. The fabrication process proposed here provides thin and lightweight energy devices with high energy and power densities. This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

S3-14: Influence of self-assembled monolayer dielectrics on network density and device performance of SWNT transistors

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Semiconducting single-walled carbon nanotube (s-SWNT) thin films are attractive materials for flexible electronics, *e.g.* in drive transistors of active-matrix displays. It is nowadays possible to separate semiconducting from metallic SWNTs by highly selective polymer-wrapping and thus create SWNT network field-effect transistors (FETs) with high carrier mobilities and high on/off ratios [1]. For the integration of SWNTs in large area electronics uniform and reproducible s-SWNT networks are required. Further, thin and high capacitance dielectrics are necessary to enable low-voltage operation and short channel FETs. Hybrid dielectrics consisting of a few nm of aluminum oxide (AlO_x) with self-assembled monolayers (SAMs) based on alkyl phosphonic acids are promising for low-voltage, bottom-gate FETs for organic semiconductors [2].

Here, we employ several AlO_x /SAM hybrid dielectrics with different head-groups (imidazolium, amine, hydroxyl and phenyl) and alkyl-chain lengths ($\text{C}_2 - \text{C}_{12}$) in FETs with solution-deposited networks of polyfluorene-wrapped large diameter s-SWNTs. We find a strong impact of the SAM headgroups on the network density for SWNT deposition by dip- and spin-coating. The FETs with gold source-drain electrodes show high on-conductances and good on/off ratios. The device parameters are relatively unaffected by the specific headgroup chemistry, which suggests a screening effect of the polymer wrapping. However, we find a distinct dependence of contact resistance on the SAMs, which limits the critical channel length. Overall, FETs with moderate SWNT coverage on SAMs with long alkyl chains and amine or hydroxyl end-groups showed the best performance with low critical channel length ($< 2 \mu\text{m}$).

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S3-15: Photonic, electronic and optoelectronic applications of polymer-sorted semiconducting carbon nanotubes

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The selective dispersion of semiconducting carbon nanotubes (s-SWNT) by wrapping with conjugated polymers has enabled their application in electronic and optoelectronic devices such as (light-emitting) field-effect transistors. The dispersion process can be easily scaled-up while maintaining good photoluminescence yield ($\sim 2.3\%$) and nanotube length ($> 1.5 \mu\text{m}$) to obtain concentrated dispersions and thin or thick films of s-SWNT with excellent optical and electrical properties. We demonstrate high mobility charge transport with high on/off ratios at low voltages and near-infrared light-emission in field-effect transistors based on monochiral and mixed networks of s-SWNT. The deliberate variation of the network composition allows us to investigate the influence of the nanotube diameter on charge transport

within the network depending on charge carrier density and temperature. Furthermore, monochiral s-SWNT films are interesting materials for strong light-matter interaction due to their small Stokes shift and large exciton binding energy. These properties enable the demonstration of exciton-polariton formation in suitable cavities and directional emission enhancement in plasmonic feedback structures.

S3-16: Scale-up fabrication of single wall carbon nanotube thin film and its application in flexible thin-film transistors

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Carbon nanotube has attracted great attention for numerous applications for future flexible electronics, owing to its supreme properties including exceptionally high electronic conductivity and mechanical strength. Carbon nanotube thin films enable the fabrication of high-performance, flexible, and transparent thin-film transistors (TFTs) with a simple transfer technique. Carbon nanotube thin films can be used not only as channel semiconductors but also as electrodes and interconnections in TFTs and integrated circuits. Here I show our progress on achieving flexible and transparent carbon nanotube thin-film transistors and integrated circuits. Carbon nanotube thin films are continuously produced by a floating-catalyst chemical vapour deposition and roll-to-roll transfer system. A simple approach to fabricate all-carbon TFTs with a photoresist as the dielectric are presented. We also proposed a method to synthesize semiconducting single-walled carbon nanotubes with a very small band-gap difference of ~ 0.08 eV showing excellent thin-film transistor performance.

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S3-17: Strong light-matter coupling of single-walled carbon nanotubes in microcavities

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For a number of emitters in the visible range, repetitive photon reabsorption in microcavities was shown to induce strong light-matter coupling and the formation of exciton-polaritons (part-light-part-matter quasiparticles). Exciton-polaritons lead to exciting phenomena, such as low-threshold lasing and Bose-Einstein condensation. In the near-infrared (NIR), however, reports of exciton-polaritons in organic materials are still missing. Interestingly, the stable NIR-luminescence of semiconducting single-walled carbon nanotubes (SWCNTs) incorporates all properties necessary for strong coupling, namely very narrow line widths, a small Stokes shift and a large oscillator strength.

Here, we show for the first time strong coupling of monochiral SWCNTs in a metal-clad microcavity at room temperature. Exciton-polaritons were unambiguously

observed in angle-resolved reflectance and polariton emission measurements that correlate well with transfer-matrix simulations. We observe the characteristic anticrossing of the cavity mode and the exciton leading to the formation of an upper and lower polariton branch. The corresponding coupling strength is determined by the mode splitting (i.e. Rabi splitting) and was measured to exceed 110 meV. Moreover, we show the transition from weak to strong light-matter coupling by varying the SWCNT concentration in the cavity.

Observation of strong coupling requires highly concentrated and monochiral SWCNT films of good optical quality. To achieve this we established high speed shear force mixing for selective dispersion of (6,5) SWCNTs with a conjugated polymer. This scalable process yields dispersions of exceptional quality, with average SWCNT tube lengths of 1.82 μm and an ensemble photoluminescence quantum yield of 2.3 %, thus outperforming conventional dispersion methods.

Our results show that SWCNTs hold great potential for further investigation and use of exciton-polariton phenomena in the NIR.

S3-18: Synthesis optimisation of SWNTs for nanoelectronic device's

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Single wall carbon nanotubes are seen as excellent candidate for application in nanoelectronic devices because of their remarkable electronic and mechanical properties [1]. These unique properties are highly dependent on their chiral structures and diameter [2]. Therefore, structure controlled growth of SWNTs, especially directly on final device's substrate, are highly desired for the fabrication of SWNT-based electronics. In this work, we present a new approach to control the diameter of SWNTs and eventually their chirality. Because of their potential to control the SWNT's chirality [3], bi-metallic nanoparticles are used to prepare alloy nanoclusters with specific structure. The catalyst nanoparticles are pre-formed following a previously described process [4]. Briefly, the oxide surface is first covered with a SAM (self-assembled monolayer) of a pyridine-functionalized silane. Then, bi-metallic (Fe-Ru, Co-Ru and Ni-Ru) complexes are assembled by coordination bonds on the pre-formed organic SAM. The resultant alloy nanoclusters are then used to catalyze SWNTs growth on SiO₂/Si substrates via CH₄/H₂ double hot-filament chemical vapor deposition (d-HFCVD). The microscopy (TEM, SEM) and spectroscopy (Raman) analysis demonstrate the high quality of SWNTs. By changing CVD temperature from 700 to 1000°C we succeeded to modulated the percentage of semi-conductor tube from 47 % to 85 %, according to Raman spectroscopy. The nanotubes were integrated into high-quality SWNT-FET with on/off ratio reaching up to seven decades.

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S3-19: The ultimate performance of single-walled carbon nanotubes as transparent conductors?

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The ultimate performance—ratio of electrical conductivity to optical absorbance—of single-walled carbon nanotube (SWCNT) transparent conductive films (TCFs) is an issue of considerable application relevance. We have in our recent report presented the first unambiguous experimental evidence that SWCNT bundling is detrimental for TCF electro-optical performance [1]. We provide an explanation of the loss in performance as an effect of gratuitous absorbance related to a greater carbon content in large diameter bundles, which is not compensated by the simultaneous gains achieved in bundle conductivity. As an outcome we present a semi-empirical absorbance-conductance model, suggesting an ultimate limit for pristine SWCNT TCF performance at $80 \Omega/\square$ at 90% transparency and for doped tubes down to $25 \Omega/\square$.

[1] Mustonen *et al.*, Uncovering the ultimate performance of single-walled carbon nanotube films as transparent conductors, *APL* 107 (2015).

S3-20: The voltage generation by movement of electrolyte solution on carbon nanotube thin film

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Energy harvesting from environment energy sources is emerging technology for driving IoT sensor devices. Recently, the voltage generation of a few millivolts from the movement of electrolyte solution have been demonstrated by using the graphene [1, 2] and a carbon nanotube (CNT) film [3]. In this work, we investigated the generation induced by the movement of electrolyte solution with highly conductive CNT thin film. The dependence of generated voltage on the CNT film thickness has also been studied. The highly conductive CNT thin films were formed on polyethylenephthalate (PEN) substrate by the dry transfer process based on the floating-catalyst chemical vapor deposition. [4]. The size of the CNT thin film was 30 mm x 4 mm. We used 2-mol/l NaCl aqueous solution as the electrolyte. The droplet of the electrolyte solution was moved on the CNT thin film by drawing. We measured voltage or current generated both ends of the CNT film. We first examined the CNT thin film of a thickness of ~ 40 nm. The open circuit voltage of 220 mV and the short circuit current of 29.3 nA was obtained when the droplet was moved on the CNT thin

film. The generated voltage was increased to 2.72 mV by decreasing the CNT film thickness to ~10 nm. This is probably due to the elimination of shunt current flowing through the underlayer CNTs.

S3-21: Voltage-driven physical gap extension of single-walled carbon nanotubes after electrical breakdown

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Electrical breakdown of single-walled carbon nanotubes (SWNTs) is widely performed to selectively cut metallic pathways in SWNT-based field-effect transistors (FETs) [1] or to fabricate nanogap electrodes [2].

Although size control of physical gaps is important in both applications, size-controlled formation of nanogaps is limited because of insufficient understanding of the size determination mechanisms. In this study, we observed voltage-driven gap extension of SWNTs on substrates after electrical breakdown, which could explain the previously reported dependence of gap size on various conditions [2]. Horizontally aligned SWNTs grown on quartz substrates were transferred onto SiO₂/Si substrates with pre-patterned metal electrodes, followed by oxygen plasma to isolate each device. Electrical breakdown was performed on a hotplate to produce small SWNT gaps. After the gap formation, voltage ramp was further applied to SWNTs with the nanogaps from 0 V to certain maximum voltages (V_{\max}). The nanogaps were extended only to anode side depending on V_{\max} and humidity. SWNTs on anode side might be electrochemically etched due to physisorbed water from air and enhanced electric field at the SWNT tips. Field emission properties were measured in vacuum as a possible charge transfer mechanism. The relation between field enhancement factor and geometrical features of SWNTs [3] well explains both voltage dependence of the extended gap size and the field emission properties of SWNT gaps. Furthermore, similar phenomena to the gap extension caused damages to adjacent SWNTs, possibly deteriorating the selectivity of electrical breakdown as cutting unwanted metallic pathways in FET channels.

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S3-22: Chirality selective synthesis of single-walled carbon nanotubes with sputtered W-based catalyst

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Single-walled carbon nanotubes (SWNTs) have been regarded as one of the most promising building-blocks in nanoelectronics due to their chirality-dependent properties. However, the potential industrial applications are impeded by the mixed chiralities of as-grown SWNT assemblies. Direct synthesis of SWNTs with single

chirality is challenging but attracts considerable attention among researchers. Catalyst plays an important role in the chirality controlled synthesis of SWNTs. Recently, Co₇W₆ clusters were reported to successfully grow a single chirality SWNT (12, 6), with over 90% abundance and a zigzag SWNT (16, 0), with near 80%, by controlling the catalyst structure and growth conditions with a high-temperature reduction and growth [1, 2].

In this report, we show that the sputtered CoW catalyst can selectively grow (12, 6) SWNTs with better uniformity by low pressure chemical vapor deposition at lower temperature [3]. The abundance of (12, 6) is over 50% according to the statistical Raman mapping analysis and optical absorption spectrum of the as-grown SWNTs. Parametric study of the CoW catalyst system demonstrates that the reduction temperature before growth is critical for the selectivity and the intermediate structure, Co₆W₆C, is identified by the electron diffraction. Moreover, the investigation of catalysts discloses the complicated structure changes before and after growth. Time-dependent selectivity and the structure evolution of catalysts will be discussed in detail.

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S3-23: Confined linear carbon chains: Synthesis and properties

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The extreme instability and strong chemical activity of carbyne, the infinite sp¹ hybridized carbon chain, are responsible for its low possibility to survive at ambient conditions. We successfully synthesized extremely long linear carbon chains (LLCCs) inside thin double walled carbon nanotubes as nanoreactors and protectors [1]. Their existence, structure, lengths and yield have been proved by Raman, HRTEM, STEM and XRD. The results show that the single-triple bonded LLCCs including thousands of carbon atoms have at least six new Raman peaks, some of which are even stronger than the G-band. The optimum growth conditions, for example, diameter of the host tubes, annealing temperatures and time were carefully studied. The interaction and charge transfer between the LLCCs and their host nanotubes were explored using

resonance Raman, low-temperature Raman and DFT calculations [2]. Furthermore, the band gap of the LLCCs was examined by resonance Raman spectroscopy. The results suggest that the band gap of LLCCs in the range of 1.8 - 2.3 eV is inversely proportional to their lengths, which is also perfectly consistent with our DFT calculations [3].

L. S., T.P. thank the FWF, P.A. acknowledges the EU.

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7th Graphene and 2D Materials Satellite Symposium	
9:00-9:05	Opening the Satellite
9:05-9:50	Key Note Lecture: Claire Berger
	<i>SiC graphene materials (S4-20)</i>
09:50-10:20	Invited Talk: Sabina Caneva
	<i>In-Situ Studies of Catalytic h-BN Growth using Synchrotron Radiation (S4-16)</i>
10:20-10:45	Coffee Break
10:45-11:30	Key Note Lecture: Jeanie Lau
	<i>Quantum transport in high mobility atomic membranes (S4-18)</i>
11:30-12:00	Invited Talk: Denis Bandurin
	<i>Experimental Evidence to the Hydrodynamic Electron Flow in Graphene (S4-9)</i>
12:00-12:15	Contributed Talk: Etienne Gaufrès
	<i>Probing the dielectric response of exfoliated black phosphorus thin layers (S4-15)</i>
12:15-12:30	Contributed Talk: Taishi Takenobu
	<i>Highly flexible and extremely high-gain complementary inverters of transition metal dichalcogenide monolayers (S4-17)</i>
12:30-13:00	Lunch
13:00-14:00	Poster Session
14:00-14:30	Invited Talk: Owen J Guy
	<i>Graphene Biosensors (S4-21)</i>
14:30-15:00	Invited Talk: Kazunari Matsuda,
	<i>Optical Properties and Application of Artificial Heterostructure using Graphene and Transition Metal Dichalcogenide (S4-22)</i>
15:00-15:15	Contributed Talk: Hiroshi Tabata
	<i>Gas-sensing response of Graphene/MoS₂ van der Waals heterostructure (S4-10)</i>
15:15-15:45	Coffee Break
15:45-16:15	Invited Talk: Vasily Perebeinos
	<i>Microscopic modeling of 2D materials (S4-19)</i>
16:15-16:30	Contributed Talk: Simone Schuler
	<i>Graphene-based photodetector on a slot waveguide (S4-12)</i>
16:30-16:45	Contributed Talk: Maria Cristina dos Santos,
	<i>Molecular adsorbates as probes of the local properties of doped graphene (S4-13)</i>
16:45-17:00	Contributed Talk: Yuki Okigawa
	<i>Effect of outgas on graphene synthesis by plasma treatment (S4-2)</i>
17:00	Closing the Satellite

Posters for GSS16: 7th Graphene and 2D Materials Satellite Symposium

S4-1: Commensurate-incommensurate phase transition in bilayers of 2D crystals

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Dislocations in layer stacking associated with boundaries between commensurate domains are known to tune graphene electronic properties. Here such dislocations in graphene and boron nitride bilayers are studied using the two-chain Frenkel-Kontorova model [1,2] on top of DFT calculations. The two-chain Frenkel-Kontorova model is extended to describe dislocations with arbitrary relative orientations of the Burgers vector, boundary between the domains and external strain. Structural transformations of bilayers in which the bottom layer is stretched and the upper one is left to relax freely are considered for increased elongation of the bottom layer. Formation energies of dislocations, dislocation width and orientation of the boundary between commensurate domains are analyzed depending on the magnitude and direction of elongation. The second-order phase transition from the commensurate phase to the incommensurate one with multiple dislocations is predicted to take place at some critical elongation. The order parameter for this transition corresponds to the density of dislocations, which grows continuously upon increasing the elongation of the bottom layer above the critical value. In graphene and metastable boron nitride with the layers aligned in the same direction, where elementary dislocations are partial, this transition, however, is preceded by formation of the first dislocation at the elongation smaller than the critical one. The phase diagrams including this intermediate state are plotted in coordinates of the magnitude and direction of elongation of the bottom layer. Bilayer graphene is found to show slightly greater critical elongations compared to boron nitride with the layers aligned in the same direction due to the higher stiffness of graphene.

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S4-2: Effect of outgas on graphene synthesis by plasma treatment

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We examine the effects of outgas from the wall of the reaction chamber on the synthesis of graphene by plasma-assisted chemical vapor deposition at low carbon concentrations. The actual partial pressures of methane and water during graphene synthesis were measured directly by mass spectrometry. The results show that actual partial pressures for respective gas species differed for each batches in spite of the same control parameters of gas supplies, which results in the graphene devices with different electrical properties. The plasma cleaning of the chamber walls prior to the graphene-synthesis increases effectively the uniformity of the electrical properties of graphene devices which is attributed to stabilization of the condition of the outgas from the chamber walls. This report is partially based on the results of a project supported by the New Energy and Industrial Technology Development Organization (NEDO).

S4-3: Growth process of h-BN in diffusion and precipitation method

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The diffusion and precipitation method is a simple solid-phase reaction one for growing atomically thin h-BN films [1-3]. A Ni foil and amorphous BN deposited on it are annealed in a vacuum. Then, B and N atoms diffuse into the foil and h-BN is precipitated on the opposite side of the foil. However, the simple bulk diffusion can not explain the mass transport because N is almost completely insoluble in Ni even at high temperature [1,2]. Thus, despite the method's simplicity, the detailed mechanisms of mass transport and h-BN formation are still open questions. Here, we studied the growth process of h-BN in the diffusion and precipitation method by SEM, AES, and EBSD. Observed shapes of BN domains were almost the same on the same Ni grain. Regular triangle-shaped domains were observed on surfaces between (111) and (001), such as a (113) face. Two orientations rotated by 60 degrees from each other were observed, as commonly seen in CVD growth. Highly strained triangle-shaped h-BN domains, which are uncommon in CVD growth, were also often observed on high index surfaces, such as a (213) face. Interestingly, orientations of strained triangle-shaped domains were almost the same, suggesting the possibility of orientation control of BN domains. Moreover, on (111) surfaces, stripe-shaped BN growths were observed. The BN stripes emerged from a grain boundary and extended to another grain boundary (the length is almost same as the Ni grain size, about 100 nm) in the (11-2) direction. Halfway before BN stripe formation, B stripes were observed. Thus, BN stripes are considered to be formed by nitridation of B stripes. Our results suggest that mass transport, especially of N atoms, is caused by grain boundary diffusion.

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S4-4: Highly flexible and extremely high-gain complementary inverters of transition metal dichalcogenide monolayers

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Monolayer transition metal dichalcogenides (TMDCs) have attracted much attention because of their large bandgap and atomically thin thicknesses and are promising semiconducting materials for future electronics. Currently, using the chemical vapor deposition (CVD) method, we synthesized various large-area TMDC monolayers and fabricated electric double layer transistors (EDLTs) in which the dielectric layers of transistors are replaced with EDLs of electrolytes.[1-8] Owing to the high specific capacitance of EDLs (1-10 $\mu\text{F}/\text{cm}^2$), EDLTs can continuously control carrier density up to $5 \times 10^{13} \text{ cm}^{-2}$, which results in the tuning of the transistor polarity between p-type and n-type. Moreover, the CVD-grown large-area TMDC monolayer EDLTs achieved a high mobility ($\sim 100 \text{ cm}^2/\text{Vs}$), high on/off ratio ($\sim 10^6$), and low S ($\sim 60 \text{ mV}/\text{dec}$). In this study, we demonstrate CMOS inverters using large-area TMDC monolayers. By combining p-type WSe₂ and n-type MoS₂ EDLTs, we fabricate CMOS inverters with the highest voltage gain among the 2D materials (~ 110), with negligible off-state voltage, large total noise margin ($> 95\%$), low power consumption ($< 200 \text{ pW}$), and good switching speed ($> 1 \text{ kHz}$). Moreover, we transfer these inverters onto plastic substrates and evaluate their bendability. The inverters on flexible substrates exhibit stable operation, even when the devices were bent to a curvature radius of 0.5 mm, thereby demonstrating highly flexible CMOS inverters of large-area TMDCs.

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[2] J.-K.Huang, T.T, L.-J.Li, et al., ACS Nano. 8, 923 (2014)

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S4-5: Patterning of plasmonic graphene nanostructures

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Nanoscale structures of graphene have different optical, electronic and plasmonic properties than intact sheets, enabling applications in electronics, photonics and optoelectronics. When it is electrically charged, graphene can also sustain plasmons that are able to be tuned with the size and shape of the structure and, unlike surface plasmons in metals, with either electrostatic doping (external voltage) or chemical doping. Localized surface plasmon resonance can be excited in graphene nanodisks in the mid-infrared (5-20 μm wavelength), and the plasmons can hybridize with phonons in adjacent materials. [1]

Spatially controlled patterning of graphene can be done with lithographic methods using a resist or alternatively particle templates as masks (colloidal lithography), but

removing these materials from the graphene surface after etching can be problematic. Due to this, cleaner graphene structures can be produced with direct writing. We use helium ion microscopy to etch plasmonic patterns to graphene, breaking its structure and with high enough dose removing the carbon layer. The nanometer-scale beam gives also a superior resolution in comparison to resist-based lithography. [2] The structures are measured with fourier transform infrared spectroscopy, using the silicon substrate as a gate electrode.

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S4-6: Air-stable carrier doping into nano-carbon materials by extraordinary molecular Lewis acid

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Graphene and carbon nanotube (CNT) thin films are expected as one of the promising materials for next-generation transparent electrodes due to their high transparency, electrical transport properties, and high flexibility. However, the sheet resistance of these nano-carbon materials is higher than that of indium tin oxide films, which is used as transparent electrodes commonly. Therefore, it is important to decrease their resistance by a chemical doping method. In addition, since chemically-doped nano-carbon films are not air-stable in previous researches, air-stable carrier dopants are strongly required for practical application [1, 2]. More concretely, in our study, we focus on the combination of the extraordinary molecular Lewis acid, diarylboronium ion (Mes_2B^+ ; Mes (mesityl) = 2, 4, 6-trimethylphenyl) and thermally-stable counter anion, tetrakis (pentafluorophenyl) borate ($[(\text{C}_6\text{F}_5)_4\text{B}]^-$) as novel air-stable dopants [3]. We prepared few-layer graphene and CNT thin films, and immersed them into the saturated o-dichlorobenzene solution of the dopants. After that, we conducted four-probe resistance, the Hall effect, thermopower and transmittance measurements for non-doped and doped films. As the results, we obtained high hole carrier density ($> 10^{14} \text{ cm}^{-2}$), strong sheet resistance reduction ($> 60\%$) and one-month air stability without significant decrease of transmittance. Importantly, the air-stability of our dopants was better than that of previous researches, such as HNO_3 , and others [1, 2]. In summary, we succeeded in air-stable hole doping into graphene and CNT thin films by the extraordinary dopants ($\text{Mes}_2\text{B}^+[(\text{C}_6\text{F}_5)_4\text{B}]^-$), which promotes the future application.

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S4-7: Bulk Direct Bandgap MoS₂ and Hot Electron Injection in Metal/MoS₂ and Metal/WSe₂ Heterojunctions

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We present a simple method using a gentle oxygen plasma treatment to produce a direct bandgap transition in many-layer MoS₂. Here, the oxygen radicals cause a slight decoupling of the layers of MoS₂, which induces an indirect-to-direct bandgap transition.¹ We observe up to a 20X increase in the photoluminescence (PL) intensity after the plasma treatment. Based on AFM measurements, we observe an increase in the interlayer separation of $\sim 1.3\text{\AA}$ per layer. DFT calculations confirm that this increase in the interlayer separation is sufficient to induce an indirect-to-direct bandgap transition. In addition, this plasma treated, many-layer MoS₂ material exhibits charge neutrality near zero gate voltage, improved mobilities, subthreshold swings, and strong circularly polarized photoluminescence.²

We will also present photoluminescence spectra of metal/MoS₂ and metal/WSe₂ heterojunctions. Here, we observe a more than 10X enhancement in the indirect band gap photoluminescence of these TMDCs deposited on various metals (e.g., Cu, Au, Ag), while the direct band gap emission remains unchanged. We believe the main mechanism of light emission arises from photoexcited hot electrons in the metal that are injected into the conduction band of MoS₂ and WSe₂ and subsequently recombine radiatively with minority holes in the TMDC.³

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S4-8: Enhanced Photocatalytic Performance of 2D Nano-kaolinite Prepared via Intercalating method for Degradation of RhB under UV Light

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2D Hexagonal nano-kaolinite was successfully exfoliated via intercalation method. Several intercalating agents such as potassium and sodium acetate, hydrazine hydrate, and potassium nitrate were studied. The resulting materials were characterized using various techniques such X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field emission-scanning electron microscope (FE-SEM), transition electron microscope (TEM), BET, photoluminescence (PL), BET surface area and UV-visible. The XRD patterns shows that the characteristic peaks of kaolinite at $2\theta = 12.3^\circ, 20.3^\circ, 24.9^\circ$ were observed. TEM and FE-SEM images show obviously a variety of morphologies, including platy, particles, booklets or sheets stacks and elongate of hexagonal kaolinite depending on the kind

of the intercalating agents. FT-IR bands display a represented band for nitrogen doping in some samples. Moreover, the data obtained from PL of the produced materials revealed that the most interested sample has the highest intensity is due to the high density of electrons that attributed to the free electrons on nitrogen atom which was detected in FTIR analysis. Surface area and band gaps are also investigated. The promising nano-kaolinite was studied for degradation of Rhodamine B dye (Rh-B) under UV light. The results revealed that a complete degradation were takes place. Several parameters for degradation such as PH, concentration of Rhodamine B dye, catalyst dose and catalyst recycling are also investigated.

S4-9: Experimental Evidence to the Hydrodynamic Electron Flow in Graphene

Bandurin, Denis (The University of Manchester, Manchester, GBR)

Theoretical and experimental studies of systems in which particles undergo frequent mutual collisions date back to more than two centuries ago. Transport in such systems is described by hydrodynamic theory that was found very successful in explaining the response of classical liquids and gases to external fields. It has been argued for a long time that collective behavior of charge carriers in solids can be also described by hydrodynamic approach. However, there has been almost no direct evidence to hydrodynamic electron transport so far. This is because the conditions at which the hydrodynamic effects become observable are very strict: the electron-electron scattering length should provide the shortest spatial scale in the problem. First of all, this requires ultra clean systems where the scattering at impurities is diminished. Second, the electron-phonon scattering rate should be smaller than that of electron-electron scattering. Due to weak electron-phonon coupling high mobility graphene devices offer an ideal system to study electron hydrodynamics. To amplify the hydrodynamic effects we employed a special measurement geometry. The idea is that in case of hydrodynamic electron flow, vortices emerge in the spatial electric current distribution near the current injection contact. That results in a development of a negative voltage drop at the nearby contacts. We were able to detect such negative signal over the range of temperatures when the electronic system is in a hydrodynamic regime. Finally, we performed a rheological study of electron liquid in graphene. The electron viscosity was found to be an order of magnitude larger than that of honey which is in good agreement with many-body calculation.

S4-10: Gas-sensing response of Graphene/MoS₂ van der Waals heterostructure

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Graphene/MoS₂ heterostructures (GMHs) built by van der Waals stacking of a graphene and a MoS₂ have a Schottky barrier at their interface, which is tunable by

controlling the work function of graphene by electrostatic or chemical doping. In this paper, we represent that the Schottky barrier height (SBH) of the GMH is sensitively affected by gas adsorption on the graphene surface of the GMH, which can be used for a Shottky-type gas sensor. We fabricated the GMH device by stacking a single-layer graphene sheet on a piece of few-layer MoS₂ on the SiO₂/Si substrate and followed by depositing the source and drain electrodes on the graphene and MoS₂ sheets, respectively. Sensor response was evaluated by measuring the change in resistance of the device upon exposure to NO₂ gas (1 ppm). To eliminate the response of the regions except for the GMH, including graphene and MoS₂ regions, these regions were covered by a gas barrier layer (SU8/PMMA) in phases. Upon exposure to NO₂ gas, the device showed a significant increase in the resistance even after covering MoS₂ region, indicating an increase in the SBH of the GMH. However, after covering the whole device except for the center region of the GMH, the response in the resistance decreased drastically. Based on the above results, we concluded that only edge part of the GMH provides the SB, contributing to the sensor response.

S4-11: Giant quantum-confined Stark effect in monolayer transition metal dichalcogenides

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Optical properties of monolayer transition metal dichalcogenides (TMDCs) are attracted attention due to their quantum-confined structure. Particularly, observation of the trion at room temperature is a solid evidence of the strong confinement effect. In recent studies, optical properties of monolayer TMDCs based on the electric field or the charge carrier modulation spectroscopy are well reported [1]. However, the effect of electric field is still not understood well [2]. This work provides a direct evidence of a giant quantum-confined Stark effect in monolayer TMDCs. We fabricated an electric double layer capacitors (EDLCs) using monolayer WS₂ and MoS₂, that were synthesized by chemical vapor deposition methods on mechanically exfoliated graphite [3]. As a dielectric material, we spincoated ion gel which is the mixture of ionic liquid ([EMIM][TFSI]) and tri-block co-polymer (PS-PMMA-PS). Using these devices, we observed PL spectral redshift (~10 meV) and the applied electric field is approximately $\sim 8 \times 10^6$ V/cm. Importantly, the redshift is proportional to square of applied voltages, VG, which is a direct evidence of the quantum-confined Stark effect.

Based on the great successes in PL measurements, as an additional step, we fabricated light-emitting diodes based on electric double layer for observation of EL spectra. Two electrodes were deposited on mechanically exfoliated monolayer WSe₂ and the ion gel was spincoated on it. We successfully observed EL spectral due to excitons and trions. Very importantly, as observed in PL, EL spectra also revealed the

quadratic VG dependent redshift because of the quantum confined Stark effect. Particularly, the maximum redshift in trion peaks was approximately 40 meV, which is close to the champion record in GaAs quantum wells.

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S4-12: Graphene-based photodetector on a slot waveguide

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The integration of electrical and optical components on a single chip, favorable silicon, is a major goal in research. Thereby, a bottleneck is given by the integration of active and passive optical elements. Two-dimensional materials allow overcoming this bottleneck and paving the way for compact integrated optical communication systems. In 2004, Geim and Novoselov discovered graphene, the two-dimensional form of carbon [1]. Since then, graphene and related materials gain a lot of attraction. Properties such as high electron mobility, high thermal conductivity and broadband absorption, to name only a few, make graphene suitable for a wide range of applications. Graphene has already been proven to be an attractive material for photodetection [2]. The integration of a graphene photodetector on an optical waveguide was shown [3]. By using a waveguide structure, the interaction between light traveling through the waveguide and the graphene layer is enhanced, leading to a strong detector response. In order to further improve the light matter interaction, here a slot waveguide was used. A slot waveguide consists of two strips of high refractive material, typically silicon, separated by a subwavelength low refractive slot. The guided light is strongly confined in the subwavelength slot, leading to a local field enhancement [4]. This effect can be utilized to enhance the interaction with the graphene, which increases the detector response up to 4V/W (35mA/W). Since the detection concept relies on the photo-thermoelectric effect, the generated photovoltage depends on the difference of the Seebeck coefficient, which is created by applying voltage of different polarities on the high refractive strips. The 3-dB bandwidth was determined using a heterodyne measurement technique [5], where we achieved a 3dB-bandwidth of ~70GHz, restricted by the measurement setup.

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S4-13: Molecular adsorbates as probes of the local properties of doped graphene

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Graphene-based sensors are among the most promising graphene's applications. The ability to signal the presence of molecular species adsorbed on this atomically thin substrate has been explored from electric measurements to light scattering. Here we show that the adsorbed molecules can be used to sense graphene properties. The interaction of porphyrin molecules with nitrogen-doped graphene has been investigated using scanning tunneling microscopy and ab initio calculations [1,2]. Molecular manipulation was used to reveal the surface below the adsorbed molecules allowing to achieve an atomic-scale measure of the interaction of molecules with doped graphene. The adsorbate's frontier electronic states are downshifted in energy as the molecule approaches the doping site, with largest effect when the molecule sits over the nitrogen dopant. Theoretical calculations showed that, due to graphene's high polarizability, the adsorption of porphyrin induces a charge rearrangement on the substrate similar to the image charges on a metal. This charge polarization is enhanced around nitrogen site, leading to an increased interaction of molecules with their image charges on graphene. Consequently the molecular states are stabilized and shift to lower energies. These findings reveal the local variation of polarizability induced by nitrogen dopant opening new routes towards the electronic tuning of graphene.

[1] Pham V. D. et al., ACS Nano 8, 9403 (2014). [2] Pham V. D. et al., submitted.

S4-14: Obtaining Single Layer of MoS₂ by Chemical Vapor Deposition

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MoS₂ is one of the most studied transition metal dichalcogenides as it is promising candidate for many applications. However, to study its 2D physical properties, a growing protocol to obtain MoS₂ single layer with large domains remains a challenge. Here we report on atmospheric pressure CVD that can obtain monolayer flakes with domain sizes exceeding 20 μm. From characterization with X-Ray Photoelectron and Raman Spectroscopy, as well as Atomic Force Microscopy, we can conclude that MoS₂ monolayers were successfully synthesized: the surface stoichiometry was verified by X-Ray Photoelectron Spectroscopy; Raman spectra confirmed the vibrational fingerprint of MoS₂ monolayers with bands at 383 and 409 cm⁻¹ corresponding to the E_{12g} and A_{1g} vibrational modes, respectively. Atomic Force Microscopy showed that the obtained MoS₂ flakes have a height of 1 nm.

S4-15: Probing the dielectric response of exfoliated black phosphorus thin layers

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Black Phosphorus (P(black)) is a 2D semiconductor characterized by a direct band gap associated to high carriers mobility. Studying pristine thin layers of P(black) is however challenging due to its strong degradation through a thickness dependent photo-assisted oxidation reaction by adsorbed oxygen in water. On the basis of such experiments, we have proposed an oxidation mechanism involving electron transfer processes based on quantum confinement and found appropriate manipulation procedures opening a route to first Raman measurements on 1 to 5 pristine layers of P(black) [1]. We use also low-loss-EELS spectroscopy to investigate the angular dependence in the Brillouin zone of the dielectric response of exfoliated P(black) in the range [1-40 eV], Our machine is equipped with an electrostatic monochromator operating at 80 kV and makes possible the investigation of the angular dependence of the dielectric function at a nm scale and with an energy resolution below 100 meV. Using this technique we have studied the onset of electronic excitations and the dispersion of the plasmons as a function of the q momentum for different crystallographic in plane orientations in mechanically exfoliated P(black) down to 2-3 layers. $\omega - q$ mapping recorded along the [200] and [002] q -directions reveals a large dispersion of the plasmon peak occurring at 19 eV at $q=0$. Q dependences along different in plane directions of the layers, clearly reveal high anisotropy effects, which are discussed with the help of suitable *ab initio* calculations.

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[2] E. Gaufrès, F. Fossard et al, in preparation

S4-16: In-Situ Studies of Catalytic h-BN Growth using Synchrotron Radiation

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Hexagonal boron nitride (h-BN) is an atomically-thin insulator with highly interesting properties as barrier-, spacer- or support-layer for future integrated electronics and photonics. Catalytic chemical vapor deposition (CVD) has emerged as the most promising route towards 'electronic-grade' h-BN films owing to its ability to produce high-quality layers over large areas, while being scalable and cost-effective. To date, h-BN CVD has been demonstrated on a range of polycrystalline metal foils and films, however, with the limited understanding of the underlying growth mechanisms under realistic processing conditions, growth control remains

rudimentary. Here, we elucidate the key role of the catalyst bulk reservoir in the Fe-catalyzed CVD of h-BN [1]. Our comparative study of Fe foils annealed in either H₂ or NH₃ prior to growth demonstrates that the preannealing atmosphere strongly alters the Fe bulk phase evolution and subsequent B/N uptake mechanisms during precursor exposure, which in turn determines the coverage, thickness and uniformity of h-BN domains. Using in-situ XRD and in-situ XPS, we monitor the structural and chemical changes induced by the reaction atmosphere and rationally engineer a prefilled Fe catalyst to achieve better growth control. We show that NH₃-preannealed Fe foils enable growth of uniform monolayer h-BN, due to a N bulk-filling effect, which limits B and N diffusion into the catalyst during exposure to borazine and reduces the incubation time for h-BN nucleation. These effects act to minimize isothermal multilayer growth and suppress additional layer formation on cooling. We thus highlight the critical and controllable contribution of the catalyst bulk in CVD-based synthesis, providing a general growth rationale that can be applied to the wider class of layered compound materials. The catalyst bulk filling method presented here provides an elegant alternative to using different catalysts or using catalyst alloying [2] to control the solubility and permeability of the growth species.

[1] Caneva et al., Nano Letters, 16, pp.1250-1261 (2016)

[2] Caneva et al., Nano Letters 15, pp. 1867-1875 (2015)

S4-17: Highly flexible and extremely high-gain complementary inverters of transition metal dichalcogenide monolayers

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Monolayer transition metal dichalcogenides (TMDCs) have attracted much attention because of their large bandgap and atomically thin thicknesses and are promising semiconducting materials for future electronics. Currently, using the chemical vapor deposition (CVD) method, we synthesized various large-area TMDC monolayers and fabricated electric double layer transistors (EDLTs) in which the dielectric layers of transistors are replaced with EDLs of electrolytes.[1-8] Owing to the high specific capacitance of EDLs (1-10 $\mu\text{F}/\text{cm}^2$), EDLTs can continuously control carrier density up to $5 \times 10^{13} \text{ cm}^{-2}$, which results in the tuning of the transistor polarity between p-type and n-type. Moreover, the CVD-grown large-area TMDC monolayer EDLTs achieved a high mobility ($\sim 100 \text{ cm}^2/\text{Vs}$), high on/off ratio ($\sim 10^6$), and low S ($\sim 60 \text{ mV}/\text{dec}$). In this study, we demonstrate CMOS inverters using large-area TMDC monolayers. By combining p-type WSe₂ and n-type MoS₂ EDLTs, we fabricate CMOS inverters with the highest voltage gain among the 2D materials (~ 110), with negligible off-state voltage, large total noise margin ($> 95\%$), low power consumption ($< 200 \text{ pW}$), and good switching speed ($> 1 \text{ kHz}$). Moreover, we transfer these inverters onto plastic substrates and evaluate their bendability. The inverters on flexible substrates exhibit stable operation, even when the devices were bent to a curvature radius of 0.5 mm, thereby demonstrating highly flexible CMOS inverters of large-area TMDCs.

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S4-18: Quantum transport in high mobility atomic membranes

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Two-dimensional membranes have emerged as fascinating platforms for investigating electronic interactions as well as quantum Hall (QH) physics. In few-layer graphene, the presence of spin and valley degrees of freedom leads to SU(4) symmetries that do not have counterparts in traditional two-dimensional electron gas based on GaAs heterostructures. The addition of layers and multiple bands with non-trivial Berry curvatures provide additional degrees of freedom, resulting in an incredibly rich display of symmetries that can be broken either spontaneously or by external scalar or gauge fields. Here I will discuss the tunable symmetries of integer and fractional quantum Hall states and the rich phase diagrams at the charge neutrality point in few-layer graphene. In few-layer black phosphorus, Shubnikov de Haas oscillations and quantum Hall states are observed. Lastly, I will discuss the superior current-carrying capacity of carbon nanotube "hotdogs".

S4-19: Microscopic modeling of 2D materials

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In recent years, 2D materials, such as black phosphorus and transition metal dichalcogenides, have attracted much attention due to their excellent transport and optical properties. Using a tight-binding model of the electron-phonon interaction we explore phonon limited mobility in black phosphorous monolayer as a function of temperature, doping and electric field. By solving Bethe-Salpeter equation, we investigate optical and excitonic properties of MoS2 monolayers in an applied in-plane electric field. We predict a quadratic Stark shift and field ionization rate and their scaling with the exciton binding energy, determined by the dielectric environment.

- [1] V. Perebeinos and J. Tersoff, Nano Lett. 14, 4376 (2014).
- [2] V. Perebeinos and J. Tersoff, Phys. Rev. Lett. 114, 085501 (2015).

S4-20: SiC graphene materials

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Epitaxial graphene on SiC presents a range of unmatched properties. With its textbook graphene band structure, large structural coherence lengths, high electronic mobility, spin diffusion lengths over hundreds of microns, wafer size scalability with no transfer, epitaxial graphene is identified both as an ideal test bed for fundamental graphene research and the best candidate for graphene-based next generation

electronics. Techniques have been invented [1] to directly grow graphene nanostructures into shape at high temperature, explicitly avoiding graphene patterning that is known to greatly affect transport properties on the nanoscale. Such produced epitaxial graphene nanoribbons (about 40nm wide) present exceptional ballistic transport properties over more than 15 μm at room temperature [2] and behave as electronic waveguides or quantum dots. Arrays of thousands of parallel graphene nanoribbons, rings and more complex structures can be similarly produced at the wafer scale. An integration strategy with Si wafer is also demonstrated.

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[2] J. Baringhaus et al. *Nature* 506, 349 (2014).

S4-21: Graphene Biosensors

Owen J. Guy

S4-22 Optical Properties and Application of Artificial Hetero-structure using Graphene and Transition Metal Dichalcogenide

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Very thin materials with a few atomic layer thickness, such as nano-carbon and atomically thin two-dimensional (2D) materials, i.e. carbon nanotube, graphene and transition metal dichalcogenide, have intensively studied from viewpoint of fundamental physics and optical application. The artificial Van der Waals hetero-structures (vdWHs) using 2D materials would show the novel optical properties, and are also key structures for realization of optical application. Here, we investigated the fundamental optical properties in vdWH. The change of excitonic behavior from intra-layer exciton to inter-layer exciton is observed in 1L-MoS₂/1L-MoSe₂ vdWH. We also studied that the photovoltaic performances of graphene/Si Schottky junction solar cells were significantly improved by inserting a CVD-grown, large MoS₂ thin-film layer. A high photovoltaic conversion efficiency is achieved with the optimized trilayer-graphene/MoS₂/n-Si solar cell.

10th International Workshop on Metrology, Standardization and Industrial Quality of Nanotubes	
9:00-9:05	Opening the Satellite
9:05-9:30	Invited Talk: Yanmei Piao <i>All is not yet solved in the resonant Raman spectroscopy in carbon nanotubes (S5-25)</i>
9:30-9:55	Invited Talk: Kaihui Liu <i>Optical Spectroscopy of Individual Nano-materials with Defined Atomic Structure (S5-24)</i>
9:55-10:05	Contributed Talk: Stein Van Bezouw <i>Encapsulation of dipolar molecules inside carbon nanotubes for nonlinear optics (S5-1)</i>
10:05-10:30	Invited Talk: Thomas Pichler <i>High resolution EELS as tool to directly correlate local structure, electronic transport and optical properties of individual SWCNT (S5-20)</i>
10:30-11:00	Coffee Break
11:00-11:25	Invited Talk: Hui Ming Cheng <i>Thermal and Electrical Transport Properties of Graphene Films Tailored by Grain Size Engineering (S5-19)</i>
11:25-11:35	Contributed Talk: Deniz Cakir <i>In situ monitoring of the effect of oxidation on the Raman signal of Graphene on Copper (S5-11)</i>
11:35-11:45	Contributed Talk: Ado Jorio <i>Raman spectroscopy to differentiate between point-like and line-like defects in graphene materials (S5-3)</i>
11:45-11:55	Contributed Talk: Krister Svensson <i>Quantifying the crystallinity of carbon nanotube materials (S5-12)</i>
11:55-12:20	Invited Talk: Fei Wei <i>Interwall Friction and Sliding Behavior of Centimeters Long Double-Walled Carbon Nanotubes (S5-22)</i>
12:20-13:45	Lunch
13:45-14:10	Invited Talk: Annick Loiseau, <i>Probing spectroscopic properties of BN and black phosphorus layers (S5-23)</i>
14:10-14:35	Invited Talk: Mary B. Chan-Park, <i>CNT separation by charge reversal (S5-17)</i>
14:35-14:45	Contributed Talk: Bo Hou <i>The effect of catalysts and carbon feedstocks in the extended CVD for small-diameter single-walled carbon nanotubes (S5-14)</i>
14:45-14:55	Contributed Talk: Zhenxing Zhu

	<i>Wafer-scale synthesis of chiral-consistent monochromatic ultralong carbon nanotubes (S5-16)</i>
14:55-15:05	Contributed Talk: Jacques Lefebvre
	<i>Real time hyperspectroscopy for dynamical study of SWCNT dispersions (S5-13)</i>
15:05-15:35	Coffee Break
15:35-16:00	Invited Talk: Toshiya Okazaki
	<i>Characterization Methods for Carbon Nanotube Dispersions in Solvents and Polymer Matrices (S5-21)</i>
16:00-16:10	Contributed Talk: Sofie Cambré
	<i>Filling-induced shifts of the electronic transitions of SWCNTs from two-dimensional fitting of fluorescence-excitation spectra (S5-9)</i>
16:10-16:35	Invited Talk: Steve Cronin
	<i>Single CNT device based measurement of ion adsorption (S5-18)</i>
16:35-17:00	Invited Talk: Robert McSweeney
	<i>Carbon Nanotubes as Nano-electrodes for Electron Transfer at the Nanoscale (S5-6)</i>
17:00	Closing the Satellite

MSIN16: 10th International Workshop on Metrology, Standardization and Industrial Quality of Nanotubes

S5-1: Encapsulation of dipolar molecules inside carbon nanotubes for nonlinear optics

Van Bezouw, Stein (University of Antwerp, Antwerp, BEL); Cambré, Sofie (University of Antwerp, Antwerp, BEL); Campo, Jochen (University of Antwerp, Antwerp, BEL); Van Werveke, wouter (University of Antwerp, Antwerp, BEL); Beirnaert, Charlie (University of Antwerp, Antwerp, BEL); C. Verlactt, Christof (University of Antwerp, Antwerp, BEL); Cool, Pegie (University of Antwerp, Antwerp, BEL); Wenseleers, Wim (University of Antwerp, Antwerp, BEL)

The 1D character of carbon nanotubes (SWCNT) makes them ideal nanochannels for encapsulating various molecules. Previously, we have found that the spectroscopic features of SWCNTs shift when molecules are encapsulated.¹⁻⁴ Here, we present the encapsulation of elongated dipolar molecules inside the 1D SWCNT channel, which naturally align head-to-tail inside the SWCNTs,⁴ resulting in a coherent addition of directional properties, such as the second-order nonlinear optical (NLO) response. The polar alignment is demonstrated by wavelength-dependent hyper Rayleigh scattering experiments (HRS)⁵⁻⁷ (i.e. second harmonic light scattering). The newly synthesized organic nanohybrids possess a giant total dipole moment and NLO response, corresponding to ~70 identically aligned molecules. These nanohybrids form solution processible building blocks which are highly interesting for the development of electro-optic modulators and switches.

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S5-2: Influence of the Surfactant of Semiconducting Carbon Nanotube Ink on Printed Transistors

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Printed electronics is attractive because it leads to low-cost and eco-friendly device fabrication. Single walled carbon nanotubes (CNT) have great potentialities to become a key material for printed electronics. One of the important issues to utilize

CNTs in electronic application is to extract highly pure semiconducting (s-) CNTs. Some extraction techniques were developed up to date. Various kinds of surfactants were used for the extraction methods and they would be concerned with extraction mechanism. For example, the selective adsorption/desorption with agarose gel (ADG) method uses anionic surfactants, sodium dodecyl sulfate (SDS), sodium cholate, and sodium deoxycholate. The electric-field-induced layer formation (ELF) method uses nonionic surfactant of alcohol ethoxylate (AE). We have developed fabrication technologies for printed CNT thin film transistors (TFTs), and also investigated s-CNT ink properties for printed CNT TFTs. We fabricated CNT TFTs on plastic films by printing process using s-CNT ink extracted by the ADG method. The most of the TFTs had large off-currents and on/off ratios were small values. It is thought that the anionic surfactants prevented the s-CNT micelles from being adsorbed to the device surface and deteriorated TFT characteristics. Next, the surfactants of s-CNT ink were exchanged to nonionic surfactants of AE by cross-flow filtration. During filtration, the SDS concentrations of the filtrates were examined as a process monitor and the final SDS concentration of the s-CNT ink was estimated to be about 1 micro mol/L. We fabricated printed TFTs using the modified s-CNT ink. They were characterized and it was found that on/off ratio increased and device yield was improved by exchanging the surfactants.

This work is based on results obtained from a project supported by the New Energy and Industrial Technology Development Organization (NEDO).

S5-3: Raman spectroscopy to differentiate between point-like and line-like defects in graphene materials

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Raman spectroscopy has been largely used to characterize carbon nanostructures, including the presence of defects in graphene and related systems. The intensity ratio between the disorder-induced D band and the Raman allowed G band provides a metric for defect quantification. However, up to now, Raman spectroscopy has not been used to differentiate between point-like and line-like defects. Here we show it is indeed possible to make a difference. From the analysis of the D and G bands, it is possible to quantify, at the same time the amount of point defects and graphene crystallite sizes.

S5-4: Simultaneous Observation of Multiple Electronic Raman Scattering in Suspended Metallic Carbon Nanotubes

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Recently, a well-defined electronic Raman scattering (ERS) feature was observed exclusively in metallic SWNTs, and was reported to center at one nearest excitonic transition energy (either M_{ii}^+ or M_{ii}^-) and appear only between the laser line and the G-band.[1] Here, we simultaneously observe multiple ERS features resonantly

enhanced at the corresponding excitonic transition energies (both M_{ii}^+ and M_{ii}^-), and located as far as ~ 500 meV away from the excitation laser energy. We obtain a positive Fano factor in the Breit-Wigner-Fano lineshape G- band when ERS is located at the higher Raman shift side of G band. This supports that the G band asymmetry originates from the interference between discrete G band and continuous ERS.[2] The ERS features redshift upon bundling whereas the energy difference between ERS^+ and ERS^- remains constant. Based on the ERS features, 16 chiralities are assigned with confidence in the dt range of 0.8-1.6 nm, using a commercial micro-Raman spectrometer equipped with only two discrete laser lines (532 nm and 633 nm).

S5-5: The Impact of the Carbon Nanotube As-Grown State on the Ability to Design its Dispersion State

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The carbon nanotubes (CNTs) dispersion state, spanning from mono-dispersed solutions to high concentration, entangled suspensions, represents an important process step in the fabrication of most industrial application, such as printing, coating, fiber spinning, and composite materials. Here, we report that the range of allowable dispersion states for a type of CNT is determined by the as-grown state of the CNTs, i.e. individual tube structure (length, diameter, wall number, crystallinity, etc) and the assembly structure (size, density, alignment, purity). A diverse array of CNTs differing in tube and assembly structures were dispersed by different dispersion mechanisms, such as turbulent flow (wet-jet mill), cavitation (sonication) and mechanical force (beads mill). The resultant dispersion states were characterized by examining the size and morphology of the dispersed CNT aggregates as well as the stability of the dispersion. These characterizations revealed the range of allowable dispersion states based on the as-grown CNT state. In general, short CNTs assembled in lower densities, with larger diameter and increased wall number exhibited less amount of dispersion states. In contrast, long CNTs assembled in higher densities, with smaller diameter and decreased wall number showed the wider range of dispersion states. Possessing a wide range of dispersion states allowed for a wide control of dispersed CNT aggregate size and morphologies. Therefore, by combining the understanding this allowable range for a particular type of CNT with modulation in the dispersion, one can control the dispersed aggregate structure. Taken together, these results demonstrate the impact of the CNT as-grown state on the ability to design the dispersion state and act as a guide for both the scientific and industrial application of CNT dispersions. This article is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

S5-6: Carbon Nanotubes as Nano-electrodes for Electron Transfer at the Nanoscale

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Electron transfer processes play a significant role in host-guest interactions and determine physicochemical phenomena emerging at the nanoscale that can be harnessed in electronic or optical devices as well as biochemical and catalytic systems. However, accurate measurement of the amount of charge transferred between guests and nanomaterials still represents a challenge. Single-walled carbon nanotubes (SWNT) utilised in our study simultaneously as containers for molecules and nanoscale electrodes, address this challenge by enabling direct electrical contact between guest-molecules and macroscale electrodes. The exact oxidation state of the guest-molecules inserted in SWNT can thus be determined by cyclic voltammetry (CV) methods, as we demonstrate for a series of electrochemically active species with different redox potentials. Due to the electron transfer from guest-molecule to nanotube, the redox potentials ($E_{1/2}$) undergo significant changes as measured directly by CV, for the first time, revealing a striking correlation between the magnitude of perturbations in molecular orbitals caused by host SWNT and the electron-donating properties of the guest-molecule. Within a series of metallocenes studied inside SWNT, redox properties of cobaltocene, being the strongest electron donor, and ferrocene, the weakest electron donor in the series, are the most and least affected by the nanotube respectively, which is in excellent agreement with our *ab initio* density functional theory calculations. Furthermore, the shift in $E_{1/2}$ is shown to be inversely proportional to the nanotube diameter, changing by an order of magnitude when the nanotube diameter varies in the range 1.0 - 2.5 nm. We have developed an electrochemical method based on coulometry that enables the precise mapping of changes in the density of states (DOS) and the Fermi level of the host SWNT caused by electron transfer from guest-molecules. Combined with the Nernst equation, this new method allows quantification of charge transfer in the host-guest system.

S5-7: Characterization Methods for Carbon Nanotube Dispersions in Solvents and Polymer Matrices

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Carbon nanotubes (CNTs) consist of a seamless cylinder of a graphitic sheet capped by hemispherical ends composed of pentagons and hexagons. Due to their extraordinary electrical and mechanical properties, CNTs are widely regarded as very attractive nanomaterials. Actually, CNT production capacity has rapidly increased worldwide as well as the continuous growth of the numbers of CNT-related papers and patents. Most products using CNTs today incorporate CNTs from the dispersion in solvents or polymer matrices. For commercialization of these products, the physical

properties of CNTs in the dispersion or matrix must be monitored to control the qualities of the products. In this talk, we will show effective evaluation methods for the CNT dispersions in liquids and solids for fabricating the CNT composite materials with desired properties. This paper is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

S5-8: Chirality-Dependent Surfactant Interactions revealed By Systematic Ultracentrifugal and Aqueous Two-Phase Separations

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The discovery that bile salt surfactants are extraordinarily efficient at solubilizing individual, intact single-wall carbon nanotubes (SWCNTs) in water¹, soon enabled the separation of different SWCNT structures for the first time by density gradient ultracentrifugation (DGU),² and more recently also by aqueous two-phase extraction (ATP).^{3,4} Despite very nice results for a number of small diameter SWCNT chiralities that have been isolated as individual species by DGU and ATP, the underlying mechanisms are not fully understood and the number of variables to be explored and optimized is enormous, preventing a systematic extension to other chiralities.

Based on the unique capabilities of optical spectroscopy for characterizing SWCNTs, we present a systematic study of the structure sorting of DGU and ATP. We combine a direct *in situ* optical characterization of the centrifuge tubes after DGU⁵ with systematic surfactant-concentration-dependent ATP separations for different (mixed) surfactants and as such obtain a more detailed understanding of and control over both separation mechanisms. These systematic studies confirm that chirality-dependent surfactant interactions determine the separation order.

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S5-9: Filling-induced shifts of the electronic transitions of SWCNTs from two-dimensional fitting of fluorescence-excitation spectra

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Single-wall carbon nanotubes (SWCNTs) possess unique structure-dependent optical and electronic properties that are extremely sensitive to changes in their local environment.¹⁻³ Previously, we have demonstrated that the electronic transitions of

SWCNTs shift when various molecules are encapsulated inside their hollow core.³⁻⁵ Such structure-dependent electronic shifts can be experimentally measured by wavelength-dependent NIR fluorescence-excitation (PLE) spectroscopy. The accurate determination of the chirality-dependent shifts is not straightforward as it is complicated by the presence of overlapping signals from multiple chiralities, each with contributions from both excitonic and band-to-band transitions as well as phonon side bands. Therefore, especially the excitation line shape has not been modeled accurately before. We propose a dedicated empirical model for the emission and excitation spectra, allowing to accurately fit the 2D wavelength-dependent PLE data.

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This work has received funding from the ERC under Horizon 2020 (679841: ORDERin1D) and the FWO-Vlaanderen.

S5-10: Improving purity of Semiconducting CNT Ink Using Multi-Step Elution Chromatography

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Semiconducting carbon nanotubes (S-CNTs) are promising material for various applications especially for flexible electronic devices. For the practical application of S-CNT, development of high-quality and low-cost S-CNT ink is very important, because it can be used for printing electronics without any additional treatment. In this work, we have developed an improved S-CNT ink preparation method using a gel column chromatography. This method realized extremely high-purity S-CNT ink, which can highly improve the stability and transfer characteristics of thin film transistors.

Usually, in the presence of sodium dodecyl sulfate (SDS), S-CNTs are adsorbed on the dextran-based gel and then eluted by deoxycholate (DOC). In the previous method, high concentration DOC eluted S-CNTs with various diameters. In this work, we have increased the DOC concentration step by step in the elution process (multi-step elution). In this case, S-CNTs were eluted sequentially from thin- to thick-S-CNTs. Furthermore, in the several fractions, the purity of S-CNT was found to be highly improved. S-CNT ink was then prepared by replacing the surfactant to nonionic one, which showed highly stable transistor performances.

This presentation is based on results obtained from a project commissioned by the New Energy and Industrial technology Development Organization (NEDO).

S5-11: In situ monitoring of the effect of oxidation on the Raman signal of Graphene on Copper

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Raman spectroscopy is widely used to monitor the properties of graphene, *e.g.* the number of layers, the amount and nature of defects, electronic and mechanical perturbations. Raman signatures of graphene deposited on silicon wafers have been extensively studied¹⁻², in particular the effects of doping and strain on the position of the G and 2D bands³, as well as the effects of interferences in the multi-layer graphene/SiO₂/Si system on their intensities⁴. On the other hand, only a few Raman studies of graphene grown, or deposited, on copper were reported so far⁴. Extensive studies are requested to better understand the interactions between graphene and the most widely used substrate for CVD growth.

The main reasons for the lack of thorough investigations are the weak Raman signal on non-oxidized copper, its sensitivity to copper oxide, and the intense photoluminescence (PL) background which hinders the observation of the Raman signal, in particular for excitations with green lasers. Yin *et al.* proposed that the intensities of the graphene bands are modulated by interferences on the multi-layer graphene/ Cu₂O /Cu system⁵. However, no deep study of the Raman and PL signatures of the copper oxide was reported so far⁶.

Here, we report an *in situ* Raman monitoring of oxidation and reduction of copper. We study the evolution of the Raman and PL signals of copper oxide and correlate them with the position and intensity of the G and 2D bands of graphene. Results will be discussed regarding the evolution of oxide thickness, as well as doping and strain of the graphene flakes. We compare the results for as-grown CVD graphene and transferred graphene on copper substrates.

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S5-12: Quantifying the crystallinity of carbon nanotube materials

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In recent years, the knowledge of the mechanical and electrical properties of carbon nanotubes (CNT) has expanded greatly. It has also become clear that different types of CNT can have vastly different material properties, the ranges of which are

presumed to be strongly correlated with crystallinity. For example, highly crystalline nanotubes fabricated by arc-discharge methods have been shown to have a Young's modulus roughly ten times that of lower crystallinity tubes grown by chemical vapour deposition (CVD) [1]. The onset of buckling and the behavior in the buckled state is also greatly affected by the crystallinity. The onset is delayed and the relative drop in stiffness is greatly reduced for CVD grown samples [1,2].

Here we propose a simple method of quantifying the crystallinity of individual CNT by transmission electron microscope diffraction, with peak width and peak symmetry being the two main quantities. The method could be used to classify the quality of CNT resulting from different growth processes, or to quantify change of crystallinity due to external manipulation such as irradiation, thermal annealing and Joule heating.

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S5-13: Real time hyperspectroscopy for dynamical study of SWCNT dispersions

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Photoluminescence excitation (PLE) mapping represents one of the most powerful tools to characterize semiconducting SWCNTs, from exciton photophysics to chirality enrichment. The method is generally slow with several minute acquisition times, and consequently provides only static snapshots of a sample. Many studies would benefit from access to shorter timescales. In this presentation, I will show that entire PLE maps with excitation and emission wavelengths spanning 500-1000 nm and 1050-1650 nm, respectively, can be acquired at timescales under 100 ms. A few examples of titration experiments will be shown on SWCNTs wrapped with conjugated polymers. I will discuss opportunities the method offers to SWCNT metrology, specifically the quantitative determination of chirality distributions.

S5-14: The effect of catalysts and carbon feedstocks in the extended CVD for small-diameter single-walled carbon nanotubes

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In CVD growth of SWNTs, different carbon feedstocks and catalysts behave differently during the processes that limit growth rate and formation of SWNTs. Here the effect of the carbon feedstocks [Ethanol, dimethyl ether (DME) and acetonitrile] and catalysts (Fe-Co, Cu-Co and W-Co) were studied in the extended CVD. Gas-phase thermal decomposition of ethanol, DME and acetonitrile were simulated using the chemical kinetic models under various SWNTs growth conditions. In addition, the different effect on the diameter and diameter distribution of SWNTs by ethanol, DME and acetonitrile were discussed. By using Fe-Co as the catalyst, the exploration of CVD conditions over a broad range of pressure results in the efficient growth of super-

small diameter SWNTs. Cu-Co and W-Co were used to obtain chirality-specific SWNTs. By using Cu-Co catalysts, diameter distribution became narrower and (6,5) became predominant at 500 °C. On the other hand, (12,6) became predominant when the fraction of W was increased in the catalyst of W-Co. Growth of super-small diameter SWNTs and the narrower chirality distribution suggest the promising future works for application and fundamental understanding of CVD growth of SWNTs.

S5-15: Using electron diffraction as a means to evaluate Raman spectroscopy for quantification of M- or S-SWNT%

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Recently there is a growing trend of using resonance Raman technique to quantify the population of a specific type of conductivity in a bulk material. In this work, we use electron diffraction as a means to evaluate its validity. Three SWNTs samples with different diameter distributions, including a ferrocene decomposition floating catalyst chemical vapor deposition (ferrocene-FC-CVD)¹ SWNT sample and a spark-based FC-CVD (spark-FC-CVD)² sample, in addition to a NIST SWNT reference sample (RM8281), have been investigated. Raman spectroscopy study with three excitation wavelengths of 514, 633, and 785nm was performed to quantify the metallic SWNT concentrations (M%) in the samples. To evaluate the Raman results, electron diffraction (ED) technique was used to directly map the chirality distribution. In the ferrocene-FC-CVD sample, M% was estimated over 90% from Raman analysis at 633nm, but 0% at 514nm, while ED analysis gave about 24%. For the spark-FC-CVD sample, the 633nm Raman analysis led to about 55% metallic tubes, but the 514 laser resulted in less than 2% though ED analysis turned out to be 33%. In particular, the Raman assessment of the well-known (6,5)-dominated NIST reference sample at all three wavelengths of 633nm, 514nm and 785nm, however, showed a small minority of (6,5) tubes, due to the weak resonance of the (6,5) tube with any of those lasers.

To conclude, our results prove that the Raman RBM intensities depend largely on the resonant conditions at certain wavelengths, rather than simply on concentrations. Up to the resonance conditions, some majority nanotube species revealed by electron diffraction measurements induce relatively weak, or even missing RBMs, and vice versa. This certainly leads to an uncertainty over Raman spectroscopy for quantitative assessment of metallic tube concentrations calculating from the relative peak intensities.

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S5-16: Wafer-scale synthesis of chiral-consistent monochromatic ultralong carbon nanotubes

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Many products have been realized based on carbon nanotubes (CNTs) despite of insufficient use of their extreme performances owing to defects in structure. In contrast, ultralong CNTs possess theoretical properties of CNTs with macroscale length, atomically consistent perfect structure and superior properties, exhibiting intriguing potential in the next-generation high-end electronics. But a great challenge to realize large-scale application is controllable wafer-scale synthesis of ultralong CNTs. In this work, we have designed a new layered cuboid reactor (LCR) and replaced the original tube furnace with a larger muffle furnace with $1000 \times 300 \times 300$ mm³ in size, which optimized the traditional chemical vapor deposition system and released the restriction of short heating zone and small-sized substrates. With longer preheating zone, multiple commutating zone and larger growth area in design, LCR has an enlarged invariable temperature area and more uniform gas velocity distribution, favorable for wafer-scale synthesis of ultralong CNTs and more than five 4-inch wafers of ultralong CNTs were firstly synthesized simultaneously. Ultralong CNTs on these wafers could be directly observed by naked eyes in ambient conditions assisted with condensed vapor, avoiding the size constraints for samples under normal electron microscope. Furthermore, Raman spectra and Rayleigh scattering demonstrated the perfect structure of as-prepared ultralong CNTs with consistent chirality. Field effect transistors fabricated from as-prepared ultralong CNTs exhibited a high on/off ratio of 10^7 , associated with the semiconducting properties and structure perfectness of ultralong CNTs. This creatively-designed system with LCR will provide a scalable and effective route to synthesize larger-area ultralong CNTs or two-dimensional nanomaterials, enabling large-scale integrated circuits and other optoelectronic applications in the future.

S5-17: CNT separation by charge reversal

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Semiconducting (semi-) single-walled carbon nanotubes (SWNTs) must be purified of their metallic (met-) counterparts for most applications including nanoelectronics, solar cells, chemical sensors, and artificial skins. Previous bulk sorting techniques are based on subtle contrasts between properties of different nanotube/dispersing agent complexes. We developed a method which directly exploits the nanotube band structure differences. The separation approach we have invented is based on the exploitation of the selectively reversal surface charge sign on the met-SWNTs, via the pH adjustment of the surfactant dispersed SWNTs. The SWNTs dispersion was prepared based on well-known methods (such as sonication and ultracentrifugation). Leveraging on the ion-exchange chromatography techniques and our proprietary modified hydrogel beads, we are able to adsorb the met-SWNTs and the resulting eluate yields 99.94% semi-SWNTs. This facile charge sign reversal (CSR)-based sorting technique is robust and can sort SWNTs with a broad diameter range.

These sorted semi-SWNTs are widely thought to be a strong contender for next-generation printed electronic transistor materials. The mobility and on/off ratio of devices with SWNTs thin film arrays shows significant enhancement as compared to

organic semiconducting materials. To achieve stable and good performance of thin film transistors, techniques such vacuum filtration, spin-/dip- coating, spray technique, immersion and inkjet printing can be used to fabricate a uniform thin SWNTs film on the desired substrate. While the alignment of SWNTs network array can be done to improve the device performance, other parameters such as the tube length, network density, purity of the network, inter-tube junction resistance and de-bundling of the tubes affects the on/off ratio and mobility of the SWNT based FETs. Inkjet printing technology has been extensively studied for depositing thin films of diverse materials for scalable, low cost printable flexible electronics. Our findings suggested that inkjet printed CNT-TFTs using a common dielectric on flexible substrate have exhibited superior performance. We deposited a thin film of the commonly used stable and high dielectric constant (k) material Hafnium oxide (HfO_2) as gate dielectric on indium-tin-oxide-coated PET film. After patterning of Au electrodes, active channels were formed by inkjet printing of highly purified (99%) semiconducting carbon nanotube ink. The optimized inkjet printed CNT-TFTs with channel length (L) = 160 μm and channel width (W) = 60 μm exhibit outstanding effective mobility of 43 $\text{cm}^2 \text{V}^{-1}\text{s}^{-1}$ with on/off ratio $\geq 10^4$. These demonstrated high-performance inkjet printed CNT-TFTs are ready for scalable printable flexible electronics in the near future.

S5-18: Single Ion Adsorption on Individual Isolated Single Walled Carbon Nanotubes

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The detection of single ions has, for many years, been the domain of large devices such as the Geiger counter, and to date, there have been no studies investigating the effects of ions on materials and devices at the single-ion level, despite the widespread use of gaseous ions to modify material surface properties, for instance by corona discharge. Here, we report on single gaseous ion adsorption onto individual carbon nanotube field effect transistors, which, due to the severely restricted one-dimensional current path, experience discrete, quantized resistance increases of over two orders of magnitude [1]. Switching events were observed during exposure to lightly ionized nitrogen, helium, oxygen, argon and air. This is in contrast to single neutral atom adsorption detection techniques, which have shown only small, barely detectable responses. Only positive ions cause changes, by the mechanism of ion potential induced carrier depletion, which is supported by density functional and Landauer transport theory. Our observations reveal a new single-ion/CNT heterostructure with novel electronic properties, and demonstrate a powerful new system for studying ion adsorption dynamics at the single-ion level.

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S5-19: Thermal and Electrical Transport Properties of Graphene Films Tailored by Grain Size Engineering

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Theoretically, the grain boundaries (GBs) in graphene have been predicted to have significant influences on various properties of graphene. However, such influences have not been well understood experimentally, in particular on thermal and electrical transport properties, because of the difficulty in the synthesis of graphene with tunable uniform grain size that is smaller than the phonon and electron mean free paths (~ a few hundreds of nanometers). We report a chemical vapor deposition method to grow monolayer graphene films with tunable uniform grain size from ~200 nm to ~1 mm, by alternating surface adsorption and segregation processes by using Pt with medium carbon solubility as substrate. We experimentally found that the thermal conductivity of these graphene films exponentially decreases with the decrease of grain size and is independent of GB orientation with a boundary conductance of $3.0 - 4.6 \times 10^9 \text{ Wm}^{-2}\text{K}^{-1}$, while the electrical conductivity slowly decreases and strongly depends on GB orientation, which are perfectly consistent with previous theoretical predictions. These findings provide valuable information for tuning the thermal and electrical transport properties of graphene for thermoelectric applications through grain size engineering.

S5-20: High resolution EELS as tool to directly correlate local structure, electronic transport and optical properties of individual SWCNT

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Physical property of a single quantum object is governed by its precise atomic arrangement. The direct correlation of localized electronic transport and optical properties with the atomic structures has been therefore strongly desired but still limited in the theoretical studies. Here, we have for the first time examined the localized electronic/optical properties of individual SWCNT combining high-resolution EELS with high-resolution TEM.

Well separated EELS peaks are obtained from a single freestanding SWCNT with the local chiral index and unambiguously related to the van Hove singularities. They clearly vary upon the different areas even in the individual carbon nanotube. Hence, these variations in interband transitions, plasmonic behaviors, and unoccupied electronic structures are clearly attributed to the local irregular atomic arrangement such as topological defect and/or elastic bond stretching [1]. This is a crucial step in the basic description of the correlated electronic structure in these nanomaterials

allowing directly extracting for instance spatially resolved exciton binding energies, the size extension of electron–hole and electron–electron correlations, and so on. Such localized electronic properties of atomically defined SWNTs would accelerate the realization of single-molecule devices such as biosensors or transistors fabricated with well-defined SWNT segments.

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S5-21: Characterization Methods for Carbon Nanotube Dispersions in Solvents and Polymer Matrices.

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Carbon nanotubes (CNTs) consist of a seamless cylinder of a graphitic sheet capped by hemispherical ends composed of pentagons and hexagons. Due to their extraordinary electrical and mechanical properties, CNTs are widely regarded as very attractive nanomaterials. Actually, CNT production capacity has rapidly increased worldwide as well as the continuous grow of the numbers of CNT-related papers and patents. Most products using CNTs today incorporate CNTs from the dispersion in solvents or polymer matrices. For commercialization of these products, the physical properties of CNTs in the dispersion or matrix must be monitored to control the qualities of the products. In this talk, we will show effective evaluation methods for the CNT dispersions in liquids and solids for fabricating the CNT composite materials with desired properties.

This paper is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

S5-22: Interwall Friction and Sliding Behavior of Centimeters Long Double-Walled Carbon Nanotubes

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Friction and wear are two main causes of mechanical energy dissipation and component failure, especially in micro/nanomechanical systems with large surface-to-volume ratios. In the past decade there has been an increasing level of research interest regarding superlubricity^{1–5}, a phenomenon, also called structural superlubricity, in which friction almost vanishes between two incommensurate solid surfaces^{2,3}. However, all experimental structural superlubricity has been obtained on the microscale or nanoscale, and predominantly under high vacuum. Here, we show that superlubricity can be realized in centimetres-long double-walled carbon nanotubes (DWCNTs) under ambient conditions. Centimetres-long inner shells can be pulled out continuously from such nanotubes, with an intershell friction lower than 1 nN that is independent of nanotube length. The shear strength of the DWCNTs is only several pascals, four orders of magnitude lower than the lowest reported value in CNTs and graphite. The perfect structure of the ultralong DWCNTs used in our experiments is essential for macroscale superlubricity. The interwall

friction shows a linear dependence on the pullout velocity of the inner wall. The axial curvature in DWCNTs causes the significant increase of the interwall friction. The axial curvature also affects the sliding behavior of the inner wall. Compared with the axial curvature, the opening ends of DWCNTs play tiny roles in their interwall friction.

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S5-23: Probing spectroscopic properties of BN and black phosphorus layers.

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In this talk, we examine the interplay between structure and spectroscopic properties of both BN and Black Phosphorous (P(black)) mechanically exfoliated layers and how these properties can be further exploited to define the basis of a characterization metrics in 2D structures beyond graphene. Spectroscopic properties were studied using cathodoluminescence (CL) at 4K, Raman spectroscopy, HRTEM and Electron Energy Loss Spectroscopy (EELS) using a monochromated Libra 200 TEMSTEM at 80 kV.

Hexagonal boron nitride (h-BN) is a wide band gap semiconductor (~ 6.5 eV), with sp^2 hybridation, which meets a growing interest for deep UV LED and graphene and 2D materials engineering [1]. Knowing better the intrinsic properties of this material therefore highly desirable. H-BN displays original optical properties governed, in the energy range 5.5 – 6 eV, by strong excitonic effects, consisting of D and S lines [2]. Thanks to the imaging capability of the CL, emission, related to D lines, is proved to be due to structural defects identified by TEM as grain boundaries or folds. In defect free areas of thin layers, D lines completely vanish and S lines only are observed. S lines are therefore identified as the intrinsic luminescence of the material [2]. We will show how exfoliated layers could be prepared with no D band and that their S-emission dramatically changes when reducing the number of layers, providing with a signature of the 2D confinement and a metrics of the thickness dependence [3]. Low-loss-EELS is an alternative approach to the nature of electronic excitations. One can indeed access to the onset of optical transitions and investigate their angular dependence. We will show that we can probe the whole Brillouin zone of BN layers appropriately cut in a HPHT h-BN single crystal along definite crystallographic orientations and represent the plasmon dispersion as a function of the q momentum [4].

P(black) thin layers have recently raised interest for their original semi-conducting properties, such as tunable direct bandgap and high carrier mobilities. Their study is however very challenging due to its fast degradation under ambient conditions. Thanks to Raman and core-loss EELS spectroscopy, we have investigated the chemistry of degradation and shown that this phenomenon is due to a thickness dependant photo-assisted oxidation reaction with absorbed oxygen in water. This oxidation is consistent with electron transfer model based on quantum confinement. On this basis we carried out appropriate manipulation procedures opening a route to first Raman TEM and Low-loss EELS measurements on pristine mono-, bi- and multi layers, which will be discussed [5].

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S5-24: Optical Spectroscopy of Individual Nano-materials with Defined Atomic Structure.

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When the characteristic length of a material shrinks to 1 nm scale, many distinct physical phenomena, such as quantum confinement, enhanced many-body interactions and strong van der Waals inter-material couplings, will appear. To investigate these related fascinating low-dimensional physics, we need a tool to quantitatively link the atomic structures to the physical properties of very small nano-materials. In this talk, I will introduce our recently developed in-situ TEM + nanooptics technique [1,2], which combines capability of structural characterization in TEM and property characterization in nanooptics on the same individual nano-materials. Several examples of using this technique to study the physics in 1D carbon nanotube system [3-6] will be demonstrated.

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S5-25: All is not yet solved in the resonant Raman spectroscopy in carbon nanotubes

Yanmei, Piao

11th International Symposium on Computational Challenges and Tools for Nanotubes

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Author-Index

A

- Adelung, Rainer (University of Kiel, Kiel, GER) 33
- Akahane, Kouichi (National Institute of Information and Communications Technology, Koganei, Tokyo, JPN) 23
- Akiba, Sachie (Department of Applied Chemistry, Waseda Univ., Tokyo, JPN)..... 35
- Aleman, Belen (IMDEA Materials, Getafe, Madrid, ESP) 42
- Alex, Sinita (Kintech Lab Ltd, Moscow, RUS)..... 35
- Alexander, Kalinkin (Boreskov Institute of Catalysis, Novosibirsk, RUS)..... 30
- Alexander, Selyutin (Boreskov Institute of Catalysis, Novosibirsk, RUS)..... 30
- Alexander, Shmakov (Novosibirsk State University/Boreskov Institute of Catalysis, Novosibirsk, RUS)..... 30
- Alvarez, Laurent (Laboratoire Charles Coulomb, Montpellier, FRA) 231
- Amara, Hakim (LEM, Chatillon, FRA)..... 36
- An, Hua (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN) 16, 244, 253
- An, Hua (The University of Tokyo, Tokyo, JPN)..... 30
- Andrei, Khlobystov (chool of Chemistry, University of Nottingham, Nottingham, GBR) 35
- Andrei, Knizhnik (Kintech Lab Ltd, Moscow, AUT) 35
- Andrei, Popov (Institute of Spectroscopy of Russian Academy of Sciences, Troitsk, AUT) 35
- Anglaret, Eric (Laboratoire Charles Coulomb, Montpellier, FRA) 277
- ARNAULT, Jean-Charles (3CEA, Diamond Sensors Laboratory, F-91191 Gif sur Yvette, Gif sur Yvette, FRA)..... 232
- Asano, Satoshi (TASC, Tsukuba, JPN)..... 40, 277
- Asashita, Takuji (Osaka University, Suita, Osaka, JPN) 262
- Atlibatur, Rüya (Istanbul Technical University, Istanbul, TUR) 19
- Ayala, Paola (University of Vienna, Vienna, AUT) 17, 244, 254

B

- Bai, Yunxiang (Tsinghua University, Beijing , CHN) .. 18
- Baldoni, Matteo (University of Nottingham, Nottingham, GBR) 275
- Bando, Yuki (Tokyo Institute of Technology, Meguro-ku, Tokyo, JPN) 222
- Bandurin, Denis (The University of Manchester, Manchester, GBR) 262
- Bantignies, Jean-Louis (Laboratoire Charles Coulomb, Montpellier, FRA) 231
- Barshtein, Gregory (The Hebrew University-Medical School, Jerusalem, ISR) 234
- Barzegar, Hamid (Department of Physics, UC Berkeley, USA, Berkeley, USA) 8

- Bayle, Maxime (Laboratoire Charles Coulomb, Montpellier Cedex 5, FRA)277
- Beirnaert, Charlie (University of Antwerp, Antwerp, BEL) ...272
- Bellec, Amandine (Université Diderot-Paris 7, Paris, FRA)265
- Besley, Elena (University of Nottingham, Nottingham, GBR)275
- Bethge, Ole (Technische Universität Wien, Vienna, AUT)264
- BIANCO, Alberto (CNRS, IBMC, UPR 3572, F-67084 Strasbourg, Strasbourg, FRA)232
- Bianco, Alberto (CNRS, Institut de Biologie Moléculaire et Cellulaire, Laboratoire d'Immunopathologie et Chimie Thérapeutique, Strasbourg, FRA)235
- Bichara, Christophe (CNRS - U. Aix-Marseille, Marseille, FRA)36
- Blaha, Peter (Materialchemie, TU Vienna, Vienna, AUT)222
- Bokova-Sirosh, Sofya (A. M. Prokhorov General Physics Institute RAS , Moscow, RUS)30
- Boncel, Slawomir (Silesian University of Technology, Gliwice, POL)37
- Bondarev, Igor (North Carolina Central University, Durham, USA).....221
- Bouanis, Fatima (ecole polytechnique, palaiseau, FRA).....27, 251
- Bouanis, Fatima (Ecole Polytechnique, Palaiseau, FRA).....43
- Bouanis, Fatima (Laboratoire de physique des interfaces et des couches minces, Palaiseau, FRA).....39
- Briones-Leon, Antonio (Faculty of Physics, University of Vienna, Vienna, AUT) 11
- ## C
- C. Verlact, Christof (University of Antwerp, Antwerp, BEL)272
- CADARSI, Stéphanie (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA)232
- Cahangirov, Seymour (Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC & DIPC, San Sebastián, ESP) 17, 244, 254
- Cakir, Deniz (Laboratoire Charles Coulomb, Montpellier Cedex 5, FRA).....277
- Cambré, Sofie (University of Antwerp, Antwerp, BEL)..272, 276
- Cambré, Sofie (University of Antwerp, Antwerp, BEL)...276
- Campidelli, Stéphane (Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences, Gif-sur-Yvette , FRA).....231
- Campo, Jochen (University of Antwerp, Antwerp, BEL)...272
- Cassabois, Guillaume (Laboratoire Charles Coulomb, Montpellier, FRA)231
- Castan, Alice (Institut de chimie moléculaire et des matériaux d'Orsay (ICMMO), Orsay, FRA).....39
- Catala, Laure (Institut de chimie moléculaire et des matériaux d'Orsay (ICMMO), Orsay, FRA).....39
- Catala, Laure (université paris sud, Orsay, AUT).....251
- Catala, Laure (université paris sud, Orsay, FRA).....27

- Chacon, Cyril (Université Diderot-Paris 7, Paris, FRA)265
- Chamberlain, Thomas (University of Leeds, Leeds, GBR)275
- chen, tianchi (Department of Chemical Engineering, Tsinghua University, beijing, CHN).....41
- Chen, Zhongming (Department of applied chemistry, Waseda Univ., Tokyo, JPN)24
- Cheng, Guo-an (Beijing Normal University, Beijing, CHN) ...46
- Cheng, Xinlu (JPN)225
- Chiashi, Shohei (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN) 16, 244, 253
- Chiashi, Shohei (The University of Tokyo, Tokyo, JPN).. 14, 21, 38, 225, 253, 279
- Chiashi, Sohei (The University of Tokyo, Tokyo, JPN).....30
- Chikkadi, Kiran (MNS ETH Zurich, Zurich, CHE)40
- Chu, Leiqliang (National University of Singapore, Singapore, SGP)263
- Claus, Martin (Chair for Electron Device and Integrated Circuits, Dresden, GER)....224
- Cojocar, Costel Sorin (Laboratoire de physique des interfaces et des couches minces, Palaiseau, FRA).....39
- Cojocar, Costel Sorin (Laboratory of Physics of Interfaces and Thin films , Palaiseau, FRA)43
- Cojocar, Costel-Sorin (ecole polytechnique, palaiseau, FRA)27, 251
- Cool, Pegie (University of Antwerp, Antwerp, BEL) ...272
- Côté, Michel (RQMP and département de Physique, Université de Montréal, Montréal, CAN)266
- Cronin, Steve (University of Southern California, Los Angeles, USA) 261
- Cui, Kehang (The University of Tokyo, Tokyo, JPN) 30
- ## D
- Davis, E (University of Nottingham, Nottingham, GBR)275
- Defiliet, Joeri (University of Antwerp, Antwerp, BEL)...276
- Delpont, Géraud (Laboratoire Aimé Cotton, Orsay, FRA) 231
- Ding, Li (Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing, Beijing, CHN).....241
- Dobusch, Lukas (Technische Universität Wien, Vienna, AUT)264
- Domanov, Oleg (Faculty of Physics, University of Vienna, Vienna, AUT) 11
- dos Santos, Maria Cristina (Universidade de São Paulo, São Paulo, BRA).....265
- Duong, Hai (National University of Singapore, Singapore, SGP) 9
- ## E
- E. Schulz, Stefan (Fraunhofer ENAS/Center for Microtechnologies, TU Chemnitz/Center for Advancing Electronics Dresden (cfaed), Chemnitz, GER) 20
- Eda, Goki (National University of Singapore, Singapore, SGP)263
- Eisterer, Michael (Atominstut, Vienna University of Technology, Vienna, AUT) .. 11
- Elena, Obratsova (A. M. Prokhorov General Physics

Institute RAS , 38 Vavilov Street, Moscow , RUS)	30	Flygare, Mattias (Karlstad University, Karlstad, SWE)	278
Esparza-Barraza, Juan Antonio (Advanced Materials Division, IPICYT Instituto Tecnológico de Zacatecas / , Zacatecas, MEX).....	28	<u>forel, salome (ecole polytechnique, palaiseau, FRA)</u>	251
Etschel, Sebastian H (Department of Materials Science & Engineering, FAU Erlangen-Nürnberg, Erlangen, GER)	248	<u>Forel, Salome (ecole polytechnique, palaiseau, FRA)</u>	27
F		Fossard, Frédéric (CNRS-Onera, Châtillon, FRA)	266
<u>Fajardo, Juan (IPICYT, San Luis Potosi, MEX)</u>	28	Fossard, Frédéric (Laboratoire d'étude des microstructures, ONERA, Châtillon, FRA)	39
Fan, Shoushan (Tsinghua University, Beijing, CHN) ...	28	Fossard, Frederic (ONERA, Chatillon, FRA)	27, 251
Fan, Zeng (National University of Singapore, Singapore, SGP) ..	9	Francoeur, Sebastien (RQMP and département Génie Physique, Ecole Polytechnique, Montréal, CAN).....	266
Favron, Alexandre (RQMP and département de Physique, Université de Montréal, Montréal, CAN).....	266	Fréty, Nicole (Institut Charles Géhard, Montpellier, FRA)	277
Federicci, Remi (University of Antwerp, Antwerp, BEL) ...	276	<u>Fuchs, Florian (Helmholtz- Zentrum Dresden Rossendorf, Dresden, GER)</u>	224
Feng, Liangzhu (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN).....	230	<u>Fukuhara, Satoru (The University of Tokyo, Tokyo, JPN)</u>	15
<u>Ferreira, Mauro (Trinity College Dublin, Dublin)</u>	224	Fukushima, Takanori (Tokyo Institute of Technology, Yokohama, JPN)	260
Fiedler, Bodo (Technical University Hamburg-Harburg Institute of Polymer Composites, Hamburg, GER)	33	Funahashi, Kazuma (Waseda university, Tokyo, JPN)	260
FLAHAUT, Emmanuel (Institut Carnot CIRIMAT, UPS-INP- CNRS, Toulouse, FRA).....	232	Furchi, Marco Mercurio (Technische Universität Wien, Vienna, AUT)	264
<u>Flavel, Benjamin Scott (Karlsruhe Institute of Technology, Karlsruhe, GER)</u>	5, 6	Futaba, Don (1) Technology Research Association for Single Wall Carbon Nanotubes 2) National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN).....	21
Florea, Ileana (ecole polytechnique, palaiseau, FRA).....	27, 251	Futaba, Don (1) Technology Research Association for Single Wall Carbon Nanotubes 2) The National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN).....	45
Flores-Gomez, Beatriz (Advanced Materials Division, IPICYT, San Luis Potosí, MEX)	28	Futaba, Don (National Institute of Advanced Industrial	

- Science and Technology,
Tsukuba, JPN)248
- G**
- Gannott, Florentina (Institute for
Physical Chemistry,
Universität Heidelberg,
Heidelberg, GER)248
- Garlof, Svenja (Technical
University Hamburg-Harburg,
Hamburg, GER) 33
- Gather, Malte C. (University of St
Andrews, St Andrews, GBR)
.....250
- Gaufrès, Etienne (CNRS-Onera,
Châtillon, FRA)266
- Gaufrès, Etienne (Laboratoire
Charles Coulomb,
Montpellier, FRA)277
- GAUTHIER, Laury (EcoLab,
CNRS, INPT, UPS, Toulouse,
Castanet Tolosan, FRA)232
- Gelin, Maxim (TU Munchen,
Munich, GER)221
- Gemming, Sibylle (Helmholtz-
Zentrum Dresden-Rossendorf,
Dresden, GER)224
- Gessner, Thomas (Fraunhofer
ENAS, Chemnitz, GER).....226
- Gillen, Roland (TU Berlin, Berlin,
GER)220
- Gilshteyn, Evgenia (Skolkovo
Institute of Science and
Technology, Moscow, RUS) 46
- GIRARD, Hugues (CEA,
Diamond Sensors Laboratory,
F-91191 Gif sur Yvette, Gif sur
Yvette, FRA)232
- Girard, Yann (Université Diderot-
Paris 7, Paris, FRA)265
- Gordon, Nahum (Electrical
Engineering, Technion, Haifa,
ISR)25
- Gorkina, Alexandra (Skolkovo
Institute of Science and
Technology, Moscow, RUS) 46
- Gosselin, Vincent (RQMP and
département de Physique,
Université de Montréal,
Montréal, CAN)266
- Gracia-Espino, Eduardo (Umea
University, Department of
Physics, Umea, SWE)..... 8
- Graf, Arko (Heidelberg
University, Heidelberg, GER)
.....250
- Grünewald, Tilman (University of
Natural Resources and Life
Sciences Vienna, Vienna,
AUT) 12
- Grünewald, Tilman A. (University
of Natural Resources and Life
Sciences Vienna, Vienna,
AUT) 12
- Grünler, Saeideh (Department of
Materials Science &
Engineering, FAU Erlangen-
Nürnberg, Erlangen, GER)248
- Gürsel, Yesim (Istanbul Technical
University, Istanbul, TUR).. 19
- H**
- Hachiya, Soichiro (Department of
applied chemistry, Waseda
Univ., Tokyo, JPN)..... 24
- Halik, Marcus (Department of
Materials Science &
Engineering, FAU Erlangen-
Nürnberg, Erlangen, GER)248
- Haluska, Miro (Micro and
Nanosystems, ETH Zurich,
Zurich, CHE)..... 40
- Hanawa, Kenzo (SHOWA
DENKO K.K., Chiba-shi, JPN)
.....240
- Hasdeo, Eddwi H. (Tohoku
University, Sendai, JPN)...273
- Hasegawa, Kei (Department of
applied chemistry, Waseda
Univ., Tokyo, JPN)..... 24
- Hasegawa, Kei (Department of
Applied Chemistry, Waseda
Univ., Tokyo, JPN)..... 35
- Hasegawa, Masataka (AIST,
Ibaraki, JPN)260
- Hasegawa, Masataka (National
Institute of Advanced
Industrial Science and
Technology, Tsukuba, JPN)
.....257

Hata, Kenji (1) Technology Research Association for Single Wall Carbon Nanotubes 2) National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	21	<u>Hirotsu, Jun (Nagoya University, Nagoya University, JPN).....</u>	243
Hata, Kenji (1) Technology Research Association for Single Wall Carbon Nanotubes 2) The National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	45	<u>Hou, Bo (National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, JPN)</u>	21, 279
<u>Hata, Kenji (AIST - National Institute of Advanced Industrial Science and Technology, JPN).....</u>	247	<u>Hu, Dongmei (Suzhou Institute of Nanotech and Nanobionics, CAS, Suzhou, CHN)</u>	24
Hata, Kenji (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	248	Hu, Jinwen (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN).....	42
He, Maoshuai (LEM, Chatillon, FRA).....	36	Huc, Vincent (Institut de Chimie Moléculaire et des Matériaux d'Orsay, Orsay, FRA)	43
<u>Heller, Daniel (Memorial Sloan Kettering Cancer Center, New York, USA)</u>	231	Huc, Vincent (Institut de chimie moléculaire et des matériaux d'Orsay (ICMMO), Orsay, FRA).....	39
<u>Hennrich, Frank (Karlsruhe Institute of Technology, Karlsruhe, GER).....</u>	5, 6	Huc, Vincent (université paris sud, Orsay, FRA).....	27, 251
Hermann, Sascha (Fraunhofer ENAS/Center for Microtechnologies, TU Chemnitz/Center for Advancing Electronics Dresden (cfaed), Chemnitz, GER)	20	<u>Hussain, Aqeel (NanoMaterials Group, Aalto University, Espoo).....</u>	29, 246
Hideaki, Numata (Technology Research Association for Single Wall Carbon Nanotubes (TASC) / NEC Corporation, Tsukuba, JPN)	40, 277	I	
Hierold, Christofer (Micro and Nanosystems, ETH Zurich, Zurich, CHE).....	40	I. El-Dosoqy, Thanaa (Aswan University, Aswan, EGY)...	261
<u>Hirata, Eri (Department of Oral Functional Prosthodontics, Graduate School of Dental Medicine, Hokkaido University, Sapporo, JPN)</u>	235	Ibrahim, Masooma (Karlsruhe Institute of Technology, Karlsruhe, GER).....	43
		Ichikawa, Masatoshi (SHOWA DENKO K.K., Chiba-shi, JPN)	240
		Igor, Prosvirin (Boreskov Institute of Catalysis, Novosibirsk, RUS)	30
		Ikuhara, Yuichi (The University of Tokyo, Tokyo, JPN)	30
		Ileana, Florea (Laboratory of Physics of Interfaces and Thin films, Palaiseau, FRA).....	43
		Inoue, Taiki (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN).....	16, 244, 253
		<u>Inoue, Taiki (The University of Tokyo, Tokyo, JPN).....</u>	14

- Inoue, Taiki (The University of Tokyo, Tokyo, JPN).....21, 38, 253, 279
- Inoue, Takai (The University of Tokyo, Tokyo, JPN)..... 30
- Irina, Lebedeva (Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian , ESP)35
- Irwansyah (SHOWA DENKO K.K., Chiba-shi, JPN)240
- Iseki, Keizo (SHOWA DENKO K.K., Chiba-shi, JPN)240
- Ishihara, Masatou (AIST, Ibaraki, JPN)260
- Ishihara, Masatou (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)257
- Ishii, Akihiro (Institute of Engineering Innovation, The University of Tokyo, Tokyo, JPN)245
- Isoniemi, Tommi (University of Jyväskylä, Jyväskylä)259
- Iwahori, Koichiro (NIKON CORPORATION, Sagamihara, Kanagawa, JPN).....240
- Izard, Nicolas (Laboratoire Charles Coulomb, Montpellier, FRA)231, 277
- J**
- Janas, Dawid (University of Cambridge, Cambridge, GBR)33
- JANOWSKA, Izabela (ICPEES, CNRS-Université de Strasbourg, UMR 7515, Strasbourg, FRA)232
- JEONG, HYEONSU (KOREA INSTITUTE OF SCIENCE AND TECHNOLOGY, Wanju, KOR)32
- Jhih-Siang, Yang (National Taiwan University of Science and Technology, Taipei, TWN) 23
- Jiang, Hua (Aalto University School of Science, Aalto) 36
- Jiang, Hua (Department of Applied Physics, Aalto University School of Science, Espoo).....280, 281, 282
- Jiang, Hua (NanoMaterials Group, Aalto University, Espoo).....29, 246
- Johannes, Biskupek (Group of Electron Microscopy of Materials Science, Central Facility for Electron Microscopy, Ulm University, Ulm , GER) 35
- Johansson, Andreas (University of Jyväskylä, Jyväskylä) 259
- Jorio, Ado (UFMG, Belo Horizonte, BRA) 273
- Joucken, Frédéric (Université de Namur, Namur, BEL)265
- Jourdain, Vincent (Laboratoire Charles Coulomb, Montpellier, FRA)277
- Jousselme, Bruno (Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences , Gif-sur-Yvette , FRA)231
- K**
- Kaeriyama, Shoko (NIKON CORPORATION, Sagamihara, Kanagawa, JPN).....240
- Kampfmüller, Johannes (Faculty of Physics, University of Vienna, Vienna, AUT) 11
- Kanahashi, Kaito (Waseda university, Tokyo, JPN)260
- Kaneko, Toshiro (Department of engineering, Tohoku University, Sendai, JPN)..... 19
- Kang, Lixing (Suzhou Institute of Nanotech and Nanobionics, CAS, Suzhou, CHN) 26

<u>Kappes, Manfred (Karlsruhe Institute of Technology, Karlsruhe, GER)</u>	5, 6
Karatepe, Nilgün (Istanbul Technical University, Istanbul, TUR)	19
Kaskela, Antti (Aalto University, NanoMaterials Group, Espoo)	252
Kataura, Hiromichi (Nanomaterials Research Institute (NMRI), AIST, Ibaraki, JPN).....	42
Kataura, Hiromichi (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, JPN)	40, 277
Katayama, Mitsuhiro (Osaka University, Suita, Osaka, JPN)	262
Kato, Ryuichi (Technology Research Association for Single Wall Carbon Nanotubes, Tsukuba, JPN)	257
Kato, Toshiaki (Department of engineering, Tohoku University, Sendai, AUT)	19
Kato, Yuichiro (Institute of Engineering Innovation, The University of Tokyo, Tokyo, JPN)	245
Kauffmann, Yaron (Electrical Engineering, Technion, Haifa, ISR)	25
Kauppinen, Esko (Aalto University School of Science, Aalto)	36
Kauppinen, Esko (Department of Applied Physics, Aalto University School of Science, Espoo)	280, 281, 282
Kauppinen, Esko (NanoMaterials Group, Aalto University, Espoo)	29, 246
Kauppinen, Esko I. (Aalto University, NanoMaterials Group, Espoo)	252
Kauppinen, Esko I. (NanoMaterials Group, Department of Applied Physics, School of Science, Aalto University, Espoo) ...	245
Kawabata, Kosuke (Department of applied chemistry, Waseda Univ., Tokyo, JPN).....	24
Khlobystov, Andrei (University of Nottingham, Nottingham, GBR)	275
<i>Kim, Seungmin (Korea Institute of Science and Technology, Wanju, KOR)</i>	<i>32</i>
<i>Kim, Youngkwan (Korea Institute of Science and Technology, Wanju, KOR) ..</i>	<i>32</i>
Kimura, Issei (Institute of Engineering Innovation, The University of Tokyo, Tokyo, JPN)	245
Kini, Mandar (Center for Microtechnologies, TU Chemnitz, Chemnitz, GER) .	20
Kishimoto, Shigeru (Graduate School of Engineering, Nagoya University, Nagoya, JPN)..	233
Kishimoto, Shigeru (Nagoya university, Nagoya, JPN) ..	243
Kishimoto, Shigeru (Nagoya University, Nagoya, JPN)..	252
Knizhnik, Andrey (Kintech Lab Ltd., Moscow, RUS)	257
Kobashi, Kazufumi (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	248
Kobayashi, Yu (Tokyo Metropolitan University, Hachioji, JPN)	263
<u>Kolanowska, Anna (Silesian University of Technology, Gliwice, POL)</u>	<u>37</u>
Koltsova, Tatiana (Peter the Great St.Petersburg Polytechnic University, St. Petersburg, RUS)	46
<u>Kong, Jing (MIT, Cambridge, USA)</u>	<u>10</u>
Kosaka, Masaki (The University of Tokyo, Tokyo, JPN)	35

- Koshino, Mikito (Tohoku University, Sendai, JPN) ...227
- Kotakoski, Jani (University of Vienna, Vienna, AUT) 17, 244, 254
- Kotchtakov, Valeri (Electrical Engineering, Technion, Haifa, ISR)25
- Kozawa, Daichi (Waseda University, Shinjuku-ku, JPN)263
- Koziol, Krzysztof (University of Cambridge, Cambridge, GBR)33
- Krall, Michael (Technische Universität Wien, Vienna, AUT)264
- Krasnikov, Dmitry (Novosibirsk State University/Boreskov Institute of Catalysis, Novosibirsk, RUS).....30
- Krupke, Ralph (Karlsruhe Institute of Technology, Karlsruhe, GER).....5, 6
- Kubo, Osamu (Osaka University, Suita, Osaka, JPN)262
- Kumamoto, Akihito (The University of Tokyo, Tokyo, JPN)30
- Kuwahara, Yuki (AIST, TASC, Tsukuba, JPN)34
- L**
- Lagier, Laura (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA)232
- Lagoute, Jérôme (Université Diderot-Paris 7, Paris, FRA)265
- Lahjiri, Fayçal (Laboratoire Charles Coulomb, Montpellier, FRA)231
- Laiho, Patrik (Aalto University, Department of Applied Physics, Espoo) 245
- Laiho, Patrik (Aalto University, NanoMaterials Group, Espoo)252
- Laiho, Patrik (NanoMaterials Group, Aalto University, Espoo).....29, 246
- Landois, Périne (Laboratoire Charles Coulomb, Montpellier, FRA)277
- Lang, Wolfgang (Faculty of Physics, University of Vienna, Vienna, AUT) 11
- Lapin, Zachary (ETH Z"urich, Z"urich, CHE) 17, 244, 254
- Laszczyk, Karolina (Technology Research Association for Single Wall Carbon Nanotubes, Tsukuba, JPN)248
- Lauret, Jean-Sébastien (Laboratoire Aimé Cotton, Orsay, FRA)231
- Lebedev, Aleksandr (Kintech Lab Ltd., Moscow, AUT)257
- Lebedeva, Irina (Universidad del Pais Vasco UPV/EHU, San Sebastian, ESP)257
- Lebedeva, Maria (University of Oxford, Oxford, GBR)275
- Lee, Dongmyeong (Korea Institute of Science and Technology, Wanju, KOR) ..*32
- Lefebvre, Jacques (National Research Council, Ottawa, CAN) 242, 279
- Levesque, Pierre, L, (RQMP and Département de Chimie, Université de Montréal, Montréal, CAN).....266
- Li, Qingwen (Suzhou Institute of Nanotech and Nanobionics, CAS, Suzhou, CHN)24, 26
- Li, Shilong (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN).....42
- Li, Wenshan (Karlsruhe Institute of Technology, Karlsruhe, GER) 5, 6
- Li, Yan (College of Chemistry and Molecular Engineering, Peking University, Beijing, CHN).....26
- Li, Yan (Peking University, Beijing, CHN)..... 13

Li, Yan (Peking University, Beijing, CHN).....	273
Lichtenegger, Helga (University of Natural Resources and Life Sciences Vienna, Vienna, AUT)	12
<u>Lin, Jarrn-Horng (National University of Tainan, Tainan, TWN)</u>	<u>32</u>
Liu, Can (Peking University, Beijing, CHN).....	273
<u>Liu, Huaping (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN)</u>	<u>42</u>
Liu, Kaihui (Peking University, Beijing, CHN).....	22, 273
Liu, Peng (National University of Singapore, Singapore, AUT)..	9
<u>Liu, Peng (Tsinghua University, Beijing, CHN).....</u>	<u>15</u>
Liu, Wei (MNS ETH Zurich, Zurich, CHE).....	40
Liu, Zhenhong (School of Mechatronics Engineering, Nanchang University, Whisker Nanotech Co Ltd, Nanchang, CHN).....	31
Liu, Zhuang (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, AUT)	230
<u>Liu, Zhuang (Soochow University, Suzhou, CHN)</u>	<u>235</u>
Loiseau, Annick (CNRS-Onera, Châtillon, FRA)	266
Loiseau, Annick (Laboratoire d'étude des microstructures, ONERA, Châtillon, FRA).....	39
<u>Loiseau, Annick (LEM,, Chatillon, FRA)</u>	<u>36</u>
Loiseau, Annick (ONERA, Chatillon, FRA)	27, 251
López-Urías, Florentino (Advanced Materials Division, IPICYT, San Luis Potosí, MEX).....	28
<u>Louie, Steven G (University of California at Berkeley, Berkeley, USA)</u>	<u>226</u>

M

M. Abdou, Sabrine (Aswan University, Aswan, EGY)....	261
<u>M. El-Sheikh, Said (Central Metallurgical R & D Institute, Cairo, EGY).....</u>	<u>18, 261</u>
Magnin, Yann (CNRS - U. Aix-Marseille, Marseille, FRA) ..	36
<u>Malik, Sharali (Karlsruhe Institute of Technology, Karlsruhe, GER).....</u>	<u>43</u>
Maliniak, Sharon (Electrical Engineering, Technion, Haifa, ISR).....	25
Mallah, Talal (Institut de Chimie Moléculaire et des Matériaux d'Orsay, Orsay,, FRA)	43
Maniwa, Yutaka (Tokyo Metropolitan University, Hachioji, JPN)	263
<u>Marchesan, Silvia (University of Trieste, Trieste, ITA).....</u>	<u>230</u>
Martel, Richard (RQMP and Département de Chimie, Université de Montréal, Montréal, CAN).....	266
Maruyama, Shigeo (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN)	16, 244, 253
Maruyama, Shigeo (National Institute of Advanced Industrial Science and Technology , Tsukuba, Ibaraki, JPN)	21, 279
Maruyama, Shigeo (The University of Tokyo, Tokyo, JPN).....	14, 30, 38, 225, 253
Marx, Janik (Technical University Hamburg-Harburg, Hamburg, GER)	33
<u>Matsuki, Keiichiro (Waseda University, Shinjuku-ku, JPN)</u>	<u>263</u>
<u>Matsumoto, Naoyuki (1) Technology Research Association for Single Wall Carbon Nanotubes 2) The National Institute of Advanced</u>	

<u>Industrial Science and Technology, Tsukuba, JPN)</u> 45	Muñoz-Sandoval, Emilio (Advanced Materials Division, IPICYT, San Luis Potosí, MEX) 28
<u>Mcsweeney, Robert (University of Nottingham, Nottingham, GBR)</u>275	Mustonen, Kimmo (Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Vienna, AUT) ... 245
MENARD-MOYON, Cécilia (CNRS, IBMC, UPR 3572, F-67084 Strasbourg, Strasbourg, FRA).....232	<u>Mustonen, Kimmo (University of Vienna, Physics of Nanostructured Materials, Vienna, AUT)</u> 252
Meng, Peng (Beijing Normal University, Beijing, CHN) ... 46	Muyshondt, Pieter (University of Antwerp, Antwerp, BEL)... 276
Meyer, Jannik C. (University of Vienna, Vienna, AUT) 17, 244, 254	N
Mikhailchan, Anastasiia (National University of Singapore, Singapore, SGP)9	Nageeb Rashad, Mohamed (Aswan University, Aswan, EGY) 261
Milyutin, Yana (Electrical Engineering, Technion, Haifa, ISR).....25	<u>Nakanishi, Takeshi (AIST, Tsukuba, JPN)</u> 223
Miyako, Eijiro (Department of Materials and Chemistry, Nanomaterial Research Institute (NMRI), National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)235	Nakayama, Ko (Waseda university, Tokyo, JPN) 260
<u>Miyamoto, Yoshiyuki (JPN)</u> ... 225	Nakazumi, Makoto (NIKON CORPORATION, Sagami-hara, Kanagawa, JPN)..... 240
Miyata, Yasumitsu (Tokyo Metropolitan University, Hachioji, JPN).....263	Nara, Kei (NIKON CORPORATION, Sagami-hara, Kanagawa, JPN)..... 240
Miyauchi, Takuya (Waseda university, Tokyo, JPN).....260	<u>Nasibulin, Albert (Skolkovo Institute of Science and Technology, Moscow, RUS)</u> 46
<u>Motaragheb Jafarpour, Saeed (Center for Microtechnologies, TU Chemnitz, Chemnitz, GER)</u> 20	Nasibulin, Albert G. (Skolkovo Institute of Science and Technology, Moscow, RUS) 252
Mothes, Sven (Chair for Electron Device and Integrated Circuits, Dresden, GER)....224	Neumaier, Daniel (AMO GmbH, Aachen, GER) 264
MOTTIER, Antoine (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA)232	Neyts, Erik (University of Antwerp, Department of Chemistry, Research group Plasman, Wilrijk, BEL) 228
MOUCHET, Florence (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA)232	Nie, Yanyan (School of Mechatronics Engineering, Nanchang University, Whisker Nanotech Co Ltd, Nanchang, CHN)..... 31
Mueller, Thomas (Technische Universität Wien, Vienna, AUT)264	Nihey, Fumi-yuki (NEC Corporation, Tsukuba, JPN)34

Niimi, Yoshiko (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, JPN)	244	Ohyama, Shinnosuke (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN) ...	16, 244, 253
Niimi, Yoshiko (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba,, JPN)	17, 254	Oi, Kohe (Osaka University, Suita, Osaka, JPN)	262
<u>Nir, Hadar (Technion & Israel Institute of Technology, Haifa, ISR)</u>	<u>25</u>	<u>Okazaki, Toshiya (AIST, Tsukuba, JPN)</u>	<u>275</u>
Nishi, Yasutaka (NIKON CORPORATION, Sagamihara, Kanagawa, JPN)	240	Okigawa, Yuki (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	257
Nishihara, Yoshiko (Atotech Deutschland GmbH, Berlin, GER)	277	Onishi, Takeo (Nagoya University, Nagoya, JPN) ..	243
Noda, Suguru (Department of applied chemistry, Waseda Univ., Tokyo, JPN)	24	Ordokhani, Fereshteh (Istanbul Technical University, Istanbul, TUR)	19
Noda, Suguru (Department of Applied Chemistry, Waseda Univ., Tokyo, JPN)	35	Oriji, Gaku (SHOWA DENKO K.K., Chiba-shi, JPN)	240
Noda, Suguru (Waseda university, Tokyo, JPN)	260	Osawa, Toshio (Department of applied chemistry, Waseda Univ., Tokyo, JPN)	24
<u>Noda, Suguru (Waseda University, Tokyo, JPN)</u>	<u>242</u>	Oshima, Azusa (The National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	45
Novotny, Lukas (ETH Z"urich, Z"urich, CHE)	17, 244, 254	Otsuka, Keigo (The University of Tokyo, Tokyo, JPN)	14
O		<u>Otsuka, Keigo (The University of Tokyo, Tokyo, JPN)</u>	<u>38</u>
Ogawa, Yui (NTT Basic Research Labs., Atsugi, JPN)	258	<u>Otsuka, Keigo (The University of Tokyo, Tokyo, JPN)</u>	<u>253</u>
Ohno, Yutaka (Department of Electrical Engineering and Computer Science, Nagoya University, Nagoya , JPN) ..	245	P	
Ohno, Yutaka (Institute of Materials and Systems for Sustainability, Graduate School of Engineering, Nagoya University, Nagoya, JPN) ..	233	Paillet, Matthieu (Laboratoire Charles Coulomb, Montpellier, FRA)	277
Ohno, Yutaka (Nagoya University, Nagoya, JPN) ..	243, 252	<u>Panes Ruiz, Luis Antonio (Chair of Materials Science and Nanotechnology, TU Dresden, Dresden, GER)</u>	<u>247</u>
Ohta, Hiromichi (Hokkaido university, Sapporo, JPN) ..	260	Pang, Zhipeng (School of Mechantronics Engineering, Nanchang University, Nanchang, CHN)	31
		Peng, Lian-Mao (Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics,	

Peking University, Beijing, Beijing, CHN).....	241
<u>Peng, Rui (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN)</u>	230
Peterlik, Herwig (Faculty of Physics, University of Vienna, Vienna, AUT)	11
Peterlik, Herwig (University of Vienna, Vienna, AUT) 17, 244, 254	
Pham, Van Dong (Université Diderot-Paris 7, Paris, FRA)	265
Phaneuf, Anne-Laurence (RQMP and département Génie Physique, Ecole Polytechnique, Montréal, CAN)	266
Pichler, Thomas (Faculty of Physics, University of Vienna, Vienna, AUT)	11
Pichler, Thomas (University of Vienna, Vienna, AUT) 17, 244, 254	
PINELLI, Eric (EcoLab, CNRS, INPT, UPS, Toulouse, Castanet Tolosan, FRA)	232
<u>Popov, Andrey (Institute for Spectroscopy Russian Academy of Science, Moscow, RUS)</u>	257
Pospischil, Andreas (Technische Universität Wien, Vienna, AUT)	264
Powell, Annie (Karlsruhe Institute of Technology, Karlsruhe, GER).....	43
Pribat, Didier (Laboratory of Physics of Interfaces and Thin films, Palaiseau, FRA)	43
Pu, Jiang (Waseda University, Shinjuku-ku, JPN)	263
Q	
Qian, Yang (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN)	16, 244, 253
Qian, Yang (The University of Tokyo, Tokyo, JPN)	30
R	
Razin, Alexey (Electrical Engineering, Technion, Haifa, ISR).....	25
<u>Reguero, Victor (IMDEA Materials, Getafe, Madrid, ESP)</u>	42
Rennhofer, Harald (University of Natural Resources and Life Sciences Vienna, Vienna, AUT)	12
Repain, Vincent (Université Diderot-Paris 7, Paris, FRA)	265
Rohringer, Philip (University of Vienna, Vienna, AUT) 17, 244, 254	
Roman, Cosmin (MNS ETH Zurich, Zurich, CHE)	40
Rousset, Sylvie (Université Diderot-Paris 7, Paris, FRA)	265
Rubio, Angel (Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Universidad del País Vasco, CFM CSIC-UPV/EHU- MPC & DIPIC, San Sebastián, ESP)	17, 244, 254
Rubio, Angel (ZZZ)	225
Rudolf, Petra (University of Groningen, Groningen).....	265
S	
Saito, Riichiro (Tohoku University, Sendai , JPN) ..	273
<u>Saito, Susumu (Tokyo Institute of Technology, Meguro-ku, Tokyo, JPN)</u>	222
Saito, Takeshi (AIST, TASC, Tsukuba, JPN)	34
Saito, Takeshi (Nanomaterials Research Institute, AIST, Tsukuba, AUT).....	11

Saito, Takeshi (National Institute of Advanced Industrial Science and Technology , Tsukuba, FRA)	231	Schulte, Karl (Technical University Hamburg-Harburg Institute of Polymer Composites, Hamburg, GER)	33
<u>Sakurai, Masahiro (The University of Texas at Austin, Austin, Texas, USA)</u>	222	Schuster, Jörg (Fraunhofer ENAS, Chemnitz, GER).....	226
Sakurai, Shunsuke (1) Technology Research Association for Single Wall Carbon Nanotubes 2) National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN) 21		Schuster, Jörg (Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, GER)	223
Sakurai, Shunsuke (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	248	Schuster, Jörg (Fraunhofer Institute for Electronic Nano Systems, Chemnitz, GER) .	224
SARRIEU, Cyril (Institut Carnot CIRIMAT, UPS-INP-CNRS, Toulouse, FRA)	232	Schwarz, Benedikt (Technische Universität Wien, Vienna, AUT)	264
<u>Sasaki, Fusako (TASC, Tsukuba, JPN)</u>	34	Schweiger, Manuel (Institute for Physical Chemistry, Universität Heidelberg, Heidelberg, GER).....	248
Sasaki, Shogo (Tokyo Metropolitan University, Hachioji, JPN).....	263	Sekiguchi, Atsuko (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	248
Sato, Yuta (Nanomaterials Research Institute, AIST, Tsukuba, JPN)	11	Semlitsch, Karl (Secar Technologie GmbH, Hönigsberg, AUT)	12
Sato, Yuta (Osaka University, Suita, Osaka, JPN)	262	Semlitsch, Karl H. (Secar Technologie GmbH, Hönigsberg, AUT)	12
Schall, Daniel (AMO GmbH, Aachen, GER).....	264	<u>Shawky Ghareeb, Ahmed (Central Metallurgical R & D Institute, Cairo, EGY) .</u>	18, 261
<u>Schießl, Stefan Patrick (Institute for Physical Chemistry, Universität Heidelberg, Heidelberg, GER).....</u>	248	<u>Shi, Lei (University of Vienna, Vienna, AUT)</u>	17, 254
Schleife, André (University of Illinois at Urbana-Champaign, Urbana / IL, USA)	226	<u>SHI, Lei (University of Vienna, Vienna, AUT)</u>	244
Schreiber, Michael (Institute of Physics, TU Chemnitz, Chemnitz, GER)	223	Shibuta, Yasushi (The University of Tokyo, Tokyo, JPN)	15
Schreiber, Michael (Technische Universität Chemnitz, Chemnitz, GER)	226	<u>Shim, Gi Woong (KAIST, Daejeon, KOR)</u>	14
<u>Schuler, Simone (Technische Universität Wien, Vienna, AUT)</u>	264	Shimojo, Fuyuki (Kumamoto University, Kumamoto, JPN)	15
		<u>Shiozawa, Hidetsugu (Elektronische Materialeigenschaften, Wien, AUT)</u>	11

Shirae, Hiruyuki (Waseda university, Tokyo, JPN).....	260	<u>Nanchang University, Whisker Nanotech Co Ltd, Nanchang, CHN)</u>	31
Shlafma, Michael (Electrical Engineering, Technion, Haifa, ISR).....	25	Susi, Toma (University of Vienna, Physics of Nanostructured Materials, Vienna, AUT) ...	252
Shoji, Yoshiaki (Tokyo Institute of Technology, Yokohama, JPN)	260	<u>Suzuki, Satoru (NTT Basic Research Labs., Atsugi, JPN)</u>	258
Shtempluck, Oleg (Electrical Engineering, Technion, Haifa, ISR)	25	<u>Svensson, Krister (Karlstad University, Karlstad, SWE)</u>	278
Shvartsman, Leonid D (The Hebrew University, Jerusalem, ISR).....	234	<u>Syari'ati, Ali (University of Groningen, Groningen)</u>	265
<u>Singer, Gerald (University of Natural Resources and Life Sciences Vienna, Vienna, AUT)</u>	12	T	
Sinn, Gerhard (University of Natural Resources and Life Sciences Vienna, Vienna, AUT)	12	<u>Tabata, Hiroshi (Osaka University, Suita, Osaka, JPN)</u>	262
Smazna, Daria (University of Kiel , Kiel, GER)	33	Takagi, Yukai (The University of Tokyo, Tokyo, JPN)	225
Sotobayashi, Hideyuki (Aoyama Gakuin University, Sagami-hara, Kanagawa, JPN)	23	Takenobu, Taishi (Nagoya university, Nagoya, JPN) ..	260
Sporcken, Robert (Université de Namur, Namur, BEL).....	265	<u>Takenobu, Taishi (Nagoya University, Nagoya, JPN)</u> ..	259
Stöger, Werner (Secar Technologie GmbH, Hönigsberg, AUT)	12	Takenobu, Taishi (Waseda University, Shinjuku-ku, JPN)	263
Suenaga, Kazu (Nanomaterials Research Institute, AIST, Tsukuba, JPN)	11	Takezaki, Hiroki (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN)	16, 244, 253
Suenaga, Kazu (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, JPN).....	244	Takezaki, Hiroki (The University of Tokyo, Tokyo, JPN)	14
Suenaga, Kazu (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, AUT)	17, 254	Tan, Xiaofang (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN).....	230
<u>Sun, Dongming (Institute of Metal Research, Chinese Academy of Sciences, Shenyang , CHN)</u>	250	Tan, Zhi-yuan (Beijing Normal University, Beijing, CHN) ...	46
<u>Sun, Xiaogang (School of Mechatronics Engineering,</u>		<u>Tanaka, Fumiaki (Technology Research Association for Single Wall Carbon Nanotubes, Tsukuba, JPN)</u>	248
		Tanaka, Naoki (Tokyo Institute of Technology, Yokohama, JPN)	260
		Tanaka, Takeshi (National Institute of Advanced	

- Industrial Science and Technology (AIST), Tsukuba, JPN)40, 277
- tang, cheng (department of chemical engineering, Tsinghua university, beijing, CHN).....41
- Tang, Hao
(Institute of Photovoltaics, Nanchang University, Nanchang 330031, PR China, Nanchang, CHN).....31
- Teichert, Fabian (Dresden Center for Computational Materials Science (DCMS), Dresden, GER)223
- Thilo, Zoberbier (Group of Electron Microscopy of Materials Science, Central Facility for Electron Microscopy, Ulm University, Ulm , GER).....35
- Thomas, Chamberlain (School of Chemistry, University of Leeds, Leeds, GBR)35
- Tian, Ying (Department of Applied Physics, Aalto University School of Science, Espoo).....280, 281, 282
- Tian, Ying (NanoMaterials Group, Aalto University, Espoo).....29, 246
- Tolochko, Oleg (Peter the Great St.Petersburg Polytechnic University, St. Petersburg, RUS).....46
- Tong, Lianming (Peking University, Beijing, CHN) ...22
- Toppari, J. Jussi (University of Jyväskylä, Jyväskylä)259
- Tran, Thang (National University of Singapore, Singapore, SGP)9
- Tropf, Laura (University of St Andrews, St Andrews, GBR)250
- Tsapenko, Alexey (Skolkovo Institute of Science and Technology, Moscow, RUS) 46
- Tsuji, Takashi (1) Technology Research Association for
Single Wall Carbon Nanotubes
2) National Institute of
Advanced Industrial Science
and Technology, Tsukuba,
JPN)..... 21
- ## U
- Ukai, Hiroyuki (The University of Tokyo, Tokyo, JPN)225
- Umeda, Shunichi (Aoyama Gakuin University, Sagamihara, Kanagawa, JPN) 23
- Unterlass, Miriam (Technische Universität Wien, Vienna, AUT) 12
- Unterlass, Miriam M.
(Technische Universität Wien, Vienna, AUT) 12
- Ushiyama, Takuya (Graduate School of Engineering, Nagoya University, Nagoya, JPN)..233
- Ute, Kaiser (Group of Electron Microscopy of Materials Science, Central Facility for Electron Microscopy, Ulm University, Ulm , GER) 35
- ## V
- Van Bezouw, Stein (University of Antwerp, Antwerp, BEL)...272
- Van der Elst, Domien (University of Antwerp, Antwerp, BEL) 276
- Van Werveke, wouter (University of Antwerp, Antwerp, BEL)272, 276
- VAZQUEZ, Ester (UCLM, MSOC Nanochemistry Group, DOC, IRICA, Ciudad Real, ESP) .232
- Vega, Sofia (Technological Institute of Celaya, Department of Chemical Engineering, Celaya, MEX). 44
- Vets, Charlotte (University of Antwerp, Department of Chemistry, Research group Plasmant, Wilrijk, BEL)228

Vilatela, Juan Jose (IMDEA Materials, Getafe, Madrid, ESP)	42	<u>Wei, Yang (Tsinghua University, Beijing, CHN)</u>	28
Vladimir, Kuznetsov (Novosibirsk State University/Boreskov Institute of Catalysis, Novosibirsk, RUS).....	30	Wei-Hung, Chiang (National Taiwan University of Science and Technology, Taipei, TWN)	23
W		Weinfeld, Kamira (Electrical Engineering, Technion, Haifa, ISR).....	25
<u>Wagberg, Thomas (Umea University, Department of Physics, Umea, SWE)</u>	8	Wendrinsky, Josef (Technische Universität Wien, Vienna, AUT)	12
<u>Wagner, Christian (Technische Universität Chemnitz, Chemnitz, GER)</u>	226	Wenseleers, Wim (University of Antwerp, Antwerp, BEL)..	272, 276
<u>Wang, Jiangtao (Tsinghua University, Beijing, CHN)</u> ...	37	Weschke, Eugen (BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, GER)	11
Wang, Qi (Tsinghua University, Beijing , CHN)	280	<u>Wick, Peter (Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, CHE)</u>	232
Wang, Qi (Tsinghua University, Beijing, CHN).....	47	Windberger, Ursula (Medical University of Vienna, Vienna, AUT)	12
Wang, Shengnan (NTT Basic Research Labs., Atsugi, JPN)	258	<u>Wirtz, Ludger (University of Luxembourg, Luxembourg)</u>	220
Wang, Ting (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhuo, CHN).....	230	Wu, Cheng (The University of Tokyo, Tokyo, JPN)	21, 279
Wang, Yanchun (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN)	42	Wu, Xiao-ling (Beijing Normal University, Beijing, CHN) ...	46
Wanko, Marius (Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC & DIPC, San Sebasti{a}n, ESP)	17, 244, 254	Wu, Xiaoyong (School of Mechantronics Engineering, Nanchang University, Whisker Nanotech Co Ltd, Nanchang, CHN).....	31
Wei, Fei (Department of Chemical Engineering, Tsinghua University, Beijing, CHN).....	41	X	
Wei, Fei (Tsinghua University, Beijing , CHN)	18	X Nguyen, Viet (Graduate School of Engineering, Nagoya University, Nagoya, JPN)..	233
Wei, Fei (Tsinghua University, Beijing, CHN).....	47, 280	Xia, KaiLun (Tsinghua University, Beijing , CHN) ..	18
		Xiang, Jian (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN).....	230

- Xiang, Rong (Department of Mechanical Engineering, The University of Tokyo, Tokyo, JPN) 16, 244, 253
- Xiang, Rong (The University of Tokyo, Tokyo, JPN)..... 14, 21, 279
- Xiang, Rong (The University of Tokyo, Tokyo, JPN)..... 30
- Xie, Huanhuan (Tsinghua University, Beijing, CHN) ..47, 280
- Xie, Huanhuan (Tsinghua University, Beijing, CHN) ... 18
- Xie, Sishen (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN) 42
- Xu, Bin (Department of engineering, Tohoku University, Sendai, JPN) 19
- Xu, Jun (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN). 230
- Xu, Ligeng (Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, CHN) 230
- Y**
- Yaish, Yuval (Electrical Engineering, Technion, Haifa, ISR) 25
- Yamada, Kentaro (NIKON CORPORATION, Sagamihara, Kanagawa, JPN) 240
- Yamada, Maho (2) National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN) 21
- Yamada, Takatoshi (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN) 257
- Yamada, Takeo (National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN) 248
- Yamamoto, Hideki (NTT Basic Research Labs., Atsugi, JPN) 258
- Yamamoto, Naokatsu (National Institute of Information and Communications Technology, Koganei, Tokyo, JPN) 23
- Yan, Aiming (Department of Physics, UC Berkeley, USA, Berkeley, USA) 8
- Yan, Xiao-lu (Beijing Normal University, Beijing, CHN) ... 46
- Yang, Dehua (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN) 42
- Yang, Feng (Peking University, Beijing, CHN) 26
- Yang, Juan (Peking University, Beijing, CHN) 273
- Yang, Yingjun (Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing, Beijing, CHN) 241
- Yao, Fengrui (Peking University, Beijing, CHN) 22
- Yasunishi, Tomohiro (Nagoya University, Nagoya, JPN).. 252
- Ye, Jianting (University of Groningen, Groningen)..... 265
- Yedgar, Saul (The Hebrew University-Medical School, Jerusalem, ISR) 234
- Yokoyama, Atsuro (Department of Oral Functional Prosthodontics, Graduate School of Dental Medicine, Hokkaido University, Sapporo, JPN) 235
- Yoshikawa, Ryo (The University of Tokyo, Tokyo, JPN) 225
- Yudasaka, Masako (Nanotube Research Center, National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN) 235
- Yue, Lifu (School of Mechatronics Engineering, Nanchang University, Whisker

Nanotech Co Ltd, Nanchang, CHN).....	31	Zhang, Jin (Peking University, Beijing, CHN).....	22
Yumin, Abdurrahman (University of Groningen, Groningen) .	265	<u>Zhang, Jin (Peking University, Beijing, CHN).....</u>	7
Yumura, Motoo (1) Technology Research Association for Single Wall Carbon Nanotubes		zhang, qiang (department of chemical engineering, Tsinghua University, beijing, CHN).....	41
2) The National Institute of Advanced Industrial Science and Technology, Tsukuba, JPN)	45	Zhang, Quan (Beijing Normal University, Beijing, CHN) ...	46
Z		zhang, rui (department of chemical engineering, Tsinghua University, beijing, CHN).....	41
Zakharko, Yuriy (Heidelberg University, Heidelberg, GER)	250	Zhang, Yingying (Tsinghua University, Beijing , CHN) ..	18
Zaumseil, Jana (Heidelberg University, Heidelberg, GER)	250	Zhang, Zhiyong (Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing, Beijing, CHN).....	241
Zaumseil, Jana (Institute for Physiscal Chemistry, Universität Heidelberg, Heidelberg, GER)	248	<u>Zhao, Qiuchen (Peking University, Beijing, CHN) ...</u>	22
<u>Zaumseil, Jana (UNIVERSITÄT HEIDELBERG, Heidelberg, GER)</u>	249	Zheng, Rui-ting (Beijing Normal University, Beijing, CHN) ...	46
Zechner, Georg (Faculty of Physics, University of Vienna, Vienna, AUT)	11	Zhou, Weiya (Institute of Physics, Chinese Academy of Sciences, Beijing, CHN).....	42
Zeevi, Gilad (Electrical Engineering, Technion, Haifa, ISR).....	25	Zhu, Zhenxing (Tsinghua University, Beijing , CHN) ..	18
Zettl, Alex (Department of Physics, UC Berkeley, USA, Berkeley, USA)	8	<u>Zhu, Zhenxing (Tsinghua University, Beijing, CHN) ..</u>	47, 280
Zhang, Daqi (Peking University, Beijing, CHN).....	273	Zienert, Andreas (Center for Microtechnologies (ZfM), TU Chemnitz, Chemnitz, GER)	223
Zhang, Hong (JPN).....	225	Zienert, Andreas (Center for Microtechnologies, Chemnitz, GER)	224
Zhang, Jin (Center for Nanochemistry, Peking University, Beijing, CHN) ...	26		