

# **Fourth Annual U.S. Air Force-Taiwan Nanoscience Initiative Workshop**

**University of Houston  
Houston, Texas, USA**

**February 8–9, 2007**

**Welcome to the Fourth Annual USAF-Taiwan Nanoscience Initiative Workshop.** This series of Workshops aims to provide a stimulating and thought-provoking forum for sharing the latest technical developments and ideas in nanoscience and nanotechnology. We are fortunate to have gathered here on the beautiful University of Houston campus some of the finest researchers in Taiwan and the U.S., and we hope you will enjoy the program of exciting talks and poster presentations on their latest scientific results.

Thanks to Prof. Paul Chu, Dr. Don Birx, Prof. Allan J. Jacobson, and Dr. John Bear of the University of Houston for their amazing hospitality, without which this meeting could not have occurred. We are indebted to Prof. Maw-Kuen Wu of Taiwan's Academia Sinica and Dr. Tsing-Tang Song of the National Nanotechnology Program Office for their support and guidance in developing the meeting agenda. Sincerest thanks also to Susan Butler and her wonderful staff, and Troy Christensen, at the Texas Center for Superconductivity at the University of Houston, to Takashi Makishima of USAF Asian Office of Scientific Research (AOARD), and to Chao-Lin Weh of Academia Sinica for their tireless efforts in support of this meeting. Finally, we are very grateful to the Taiwanese National Science Council and to Dr. Ken Goretti of AOARD for travel sponsorship that has made attendance at this Workshop possible for many accomplished researchers.

Thank you for your participation. We look forward to an outstanding meeting.

Sincerely,

Dr. Harold Weinstock  
Dr. Jim Chang  
Capt Joe Tringe

Program Managers, USAF Office of Scientific Research

# WORKSHOP PROGRAM

## Thursday, February 8

**07:30-08:10 Registration**  
**(Athletics/Alumni Center)**

**08:10-08:30 Opening Remarks**

*Dr. Harold Weinstock (AFRL/AFOSR),  
Prof. Paul Chu (University of Houston),  
Prof. M. K. Wu (Academia Sinica),  
Dr. Jim Chang (AFRL/AOARD), and  
Dr. Jack Agee (Rice University)*

**08:30-10:00 Session 1: Silicon  
Nanostructures**

*Capt Joe Tringe (AFOSR), Chair*

**08:30-08:50**

### **Hybrid Semiconductor/ Nanoelectronic Circuit Architectures**

**Konstantin K. Likharev**

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I will present a review of the recent work on hybrid semiconductor/nanodevice integrated circuits. Such a circuit combines a CMOS subsystem, fabricated with the usual lithographic patterning, and a nanowire crossbar with simple bistable two-terminal devices at each crosspoint, fabricated by advanced (e.g., nanoimprint) patterning. The CMOS and nano subsystems are connected with an area-distributed “CMOL” interface which allows the CMOS subsystem to address every nanodevice, even without nanoscale alignment of the two subsystems. Detailed simulations have shown that the hybrid circuits may serve as the basis for:

- (i) terabit-scale memories with access time below 100 ns and defect tolerance up to 10%,
- (ii) FPGA-like reconfigurable logic circuits with density about two orders of magnitude higher than that of CMOS FPGAs (fabricated with similar design rules), and
- (iii) mixed-signal neuromorphic networks (“CrossNets”) which may become the first hardware basis for challenging the human cerebral cortex in both areal density and speed.

Recently the work on the hybrid CMOS/nano circuits received a strong boost from the experimental demonstration of highly reproducible metal-oxide devices with the necessary functionality and nanowire crossbars with sub-30-nm half-pitch. As a result, it seems that all CMOL components are ready for the first integration attempts.

**08:50-09:10**

### **Nanocrystallite Si Based MOS Light Emitting Diodes**

**Gong-Ru Lin**

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The optical properties of a  $\text{SiO}_x$  film rapid-thermal-annealed (RTA) by  $\text{CO}_2$  laser are primarily investigated. The micro-photoluminescence ( $\mu\text{-PL}$ ) and HRTEM analysis indicate that the precipitation of random-oriented Si nanocrystals can be initiated when laser intensity ( $P_{\text{laser}}$ ) larger than  $4.5 \text{ kW/cm}^2$ . At  $P_{\text{laser}}$  of  $6 \text{ kW/cm}^2$ , the Si nanocrystals exhibits a largest diameter of 8 nm and a highest density of  $4.5 \times 10^{16} \text{ cm}^{-3}$ , which emits strong PL at 790-825 nm. The micro-photorefectance of the  $\text{CO}_2$  laser RTA  $\text{SiO}_x$  film reveals a volume-density-product dependent refractive index increasing from 1.57 to 1.87 as the  $P_{\text{laser}}$  increases from 1.5 to  $7.5 \text{ kW/cm}^2$ . Nonetheless, the laser ablation of  $\text{SiO}_x$  film occurs with a linear ablation slope of  $35 \text{ nm/kW/cm}^2$  at beyond  $7.5 \text{ kW/cm}^2$ , which terminates the enlargement of Si nanocrystals, degrades the near-infrared PL, and slightly reduces the refractive index of the  $\text{CO}_2$  laser RTA  $\text{SiO}_x$  film. With such a  $\text{CO}_2$  laser annealed  $\text{SiO}_x$  film, we are able to fabricate a metal-oxide-semiconductor light-emitting diode with turn-on voltage and current of 79 V and  $33 \text{ mA/cm}^2$ , respectively. The  $\text{CO}_2$  RTA  $\text{SiO}_x$  based MOSLED emits output power up to 29 nW with a P-I slope of P-I slope:  $4.4 \text{ mW/A}$ . We further show a preliminary data of a MOSLED grown on Si substrate with interfacial Si nano-pyramid, which further enhances the quantum efficiency to  $>10^{-4}$  and electroluminescent power of  $>0.1 \text{ }\mu\text{W}$ .

09:10–09:30

## Trigate Silicon Nanowire Transistors: The Role of Interactions

**M.J. Gilbert, D. Basu, and S.K. Banerjee**

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As the march towards ever smaller silicon devices continues unabated, we are rapidly approaching size scales where the bulk silicon transistor can no longer deliver sufficient device performance. Of the many different devices under consideration to replace the bulk silicon transistor, one of the most interesting is the nanowire transistor. Because of the size of these devices, there have been many approaches to implement full quantum mechanical simulations. To date, most of these approaches have considered only ballistic transport. In this talk, we will use the recursive scattering matrix method to calculate the three dimensional transport properties of silicon nanowire transistors in the presence of a variety of interactions including electron-impurity, electron-phonon and surface roughness scattering. We find that while it is possible to recover much of the ballistic behavior of silicon nanowire transistors in the presence of elastic scattering, the inclusion of the electron-phonon interaction significantly alters the transport characteristics.

09:30–09:45

## Si/Ge light emitters

**Chee Wee Liu**

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The Si-based photonics can not only potentially expand the functionalities of Si chips such as optical interconnect, photodetection, and light emission, but also probe the electron-photon interaction in the indirect bandgap material systems with different momentum conservation processes. The metal-insulator- semiconductor (MIS) **tunneling structure is used to introduce the electron-hole radiative recombination with the involvement of the roughness scattering, phonon scattering, and localization of carriers to reach the momentum conservation.** The MOS light emitter has the advantage of simple process without the pn junction formation. The minority carriers **tunnel from the gate electrode and recombine with the majority carriers at the insulator/semiconductor interface at accumulation bias.** By the incorporation of SiGe **quantum dots and quantum wells,** the emission wavelength can be tuned from 1.1, 1.3, and 1.5

to 2.2  $\mu\text{m}$  due to the bandgap shrinkage by the strain and Ge incorporation. The  $\sim 2 \mu\text{m}$  emission can be obtained by the type II heterojunction recombination between the Si conduction band and SiGe valence band. The external strain is used to further change the emission wavelength. The electron-hole-plasma recombination model can fit the emission spectra and extract the bandgap information. The strain-induced wavelength shift can be quantitatively understood by deformation potential theories. Similarly, a MOS type detector can be made and operated at the inversion bias. Finally, the digital communication between the MOS LEDs and MOS detectors using 1.8  $\mu\text{m}$  wavelength is demonstrated.

09:45–10:00

## Hydrophobic Fluorinated Polyhedral Oligomeric Silsesquioxanes

**Joseph M. Mabry**

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Polyhedral oligomeric silsesquioxanes (POSS) are organic/inorganic hybrid materials that contain both silicon-oxide and organic functionality. In current work, POSS building blocks seem to be non-interacting. Specifically, the organic groups surrounding the silsesquioxane core are composed of fluoroalkyl moieties. Fluoroalkyl compounds are known to be rather inert. This is largely because they are non-polarizable and have low surface free energies.

Various surface properties of the FluoroPOSS compounds have been examined. The Fluorodecyl POSS has a water contact angle of  $154^\circ$ , which is approximately  $40^\circ$  higher than the water contact angle of PTFE. However, not all FluoroPOSS compounds are so hydrophobic. Examination of crystal structures gives an indication of the reason for the difference. The molecular-scale surface roughness of the Fluorodecyl POSS is much greater than the other FluoroPOSS compounds. This nano-scale roughness, in combination with the micro-scale processing roughness, leads to the improved hydrophobicity. This may be similar to the surface found on the leaves of a Lotus plant, where nano-scale and micro-scale roughness combine to provide ultrahydrophobicity.

These materials are monodisperse and crystalline. This paper will discuss many of the parameters and properties of FluoroPOSS materials. AFM images will be used to illustrate surface roughness. Water contact angles and critical surface tension calculations will be used to describe surface properties.

Cleared as AFRL-ERS-PAS-07-017.

**10:00–10:15 Break**

**10:15–11:30 Session 2: GaN and InN Nanostructures**

*Professor Shing-Chung Wang (National Chiao Tung University), Chair*

**10:15–10:30**

**Enhanced Photoconduction and Surface Conduction in GaN and InN Nanowires**

**Kuei-Hsien Chen<sup>1,2\*</sup>, Reui-San Chen<sup>1</sup>, Hsin-Yi Chen<sup>1,3</sup>, Chien-Yao Lu<sup>1</sup>, Li-Chyong Chen<sup>2</sup>, Yang-Fang Chen<sup>2,4</sup>, Ying-Jay Yang<sup>3</sup>**

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The advent of nanotechnology brings forth materials of reduced dimensionality and size, which renders novel transport phenomena such as two-dimensional electron gas, one-dimensional Luttinger liquid, zero-dimensional Coulomb blockade, *etc.* However, it remains unclear how the carrier transport processes evolve from conventional bulk behavior to surface-controlled nature in the semiconductor nanowires beyond quantum confinement regime. In this paper, we show for the first time that a significant increase in charge collection efficiency caused by spatial separation of carriers in nanowire with reduced diameter leads to a dramatic increase in its conductance, both under dark and upon light illumination. For instance, more than 100 times enhancement in the photoconduction responsivity and gain is reported when the size of GaN nanowires is reduced from 250 to 100 nm. A new transport mechanism in nanowires based on core-shell structure is proposed. By way of photoelectrochemical surface treatment, the contribution from the shell and the core can be distinguished. It is concluded that carrier separation occurs in the photoexcited GaN nanowires with electrons and holes accumulated at the surface and the core, respectively, resulting in ultra long lifetime of the carriers. Such semiconductor nanowires with efficient charge transport and collection show great promise as functional building blocks for solar energy harvesting, sensing, photocatalytic, and photochemical devices.

**10:30–10:45**

**Optimized structure design for high extraction efficiency LED Growth on pattern substr**

**Jung-Min Hwang<sup>1,3,a</sup>, Yu-Zong Shu<sup>1</sup>, Kei-May Lau<sup>2,b</sup> and Huey-Liang Hwang<sup>1,c</sup>**

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Recently, high efficiency white LEDs have gained much interest because the replacement of fluorescent lamps could be realized in the near future. Nowadays the high values of internal extraction efficiency have already been obtained because of the mature growth of epitaxy technology. However, the light extraction efficiency is always small due to the total internal reflection effect. In order to enhance the light extraction efficiency of a high power operated flip-chip LED, we designed the different patterned structures between the sapphire layer and GaN layer. The patterned surface can reduce the total internal reflection and increase the probability of light escaping from the chip. In this work we designed different patterned surfaces to simulate the enhancement of light extraction efficiency of a GaN based flip-chip LED. The ray-tracing software employed the Monte-Carlo algorithm for ray-tracing. The optimized structure for high extraction efficiency LED growth on pattern substrate was designed. The basic model in the simulation is a GaN based flip-chip LED. The flip-chip consists of a sapphire layer and a GaN/n-GaN/InGaN MQW/p-GaN layers. Part of the InGaN MQW layer and the p-GaN layer are removed to expose the n-GaN layer, and the n-type contacts are formed on the region. Under the p-GaN layer, there is a thick p-type contact which acts as a reflective mirror. Lastly the chip is soldered to a silicon sub-mount.

The actual structure sizes and optical properties of each layer are specified. The chip area is 338x358  $\mu\text{m}^2$  and the peak wavelength of the light is 470nm. In addition, in the electron-hole pairs recombination process, the light rays were generated in the active layer of LED with a uniform random distribution. So we set the light source of the flip-chip model with a uniform distribution and site on the top surface and bottom surface of the active layer. Based on the model, we designed different rough structures between the sapphire layer and GaN layer in the simulation.

10:45–11:00

## GaN Overgrowth on GaN Nanocolumns by Molecular Beam Epitaxy

**J. D. Albrecht and R. Cortez**

*Air Force Research Laboratory, Sensors Directorate, WPAFB, OH*

**K. Averett, J. E. Van Nostrand, and J. Boeckl**

*Air Force Research Laboratory, Materials and Manufacturing Directorate, WPAFB, OH*

**C.C. Yang**

*Graduate Institute of Electro-Optical Engineering and Department of Electrical Engineering, National Taiwan University, Taipei, Taiwan*

GaN nanocolumns grown by plasma-assisted molecular beam epitaxy are explored as host structures for overgrowth of bulk-like GaN films. We investigate the layers of vertical GaN nanocolumns 90+/-10 nm in width which were grown on Al<sub>2</sub>O<sub>3</sub>(0001) and Si(111) substrates. We present photoluminescence, x-ray diffraction, and microscopy data that indicates that the columns are unstrained, low-defect wurtzite GaN nanostructures. The nanocolumns form discontinuous layers with areal densities controlled by grown conditions. The nanocolumn layers are subsequently overgrown with thick GaN films and compared with commercial GaN template materials used for device fabrication. The overgrowth of GaN is studied as a function Ga flux and growth temperature. We present photoluminescence and Hall effect characterization of the overgrown layers. The microstructure and morphology are probed by atomic force and transmission electron microscopy, as well as x-ray diffraction.

Cleared as AFRL-WS 05-2768.

11:00–11:15

## Spin-splitting 2DEG in Al<sub>x</sub>Ga<sub>1-x</sub>N/GaN and its application

**Ikai Lo**

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We observed the beating pattern of Shubnikov-de Haas (SdH) oscillations for 2DEG in AlGa<sub>x</sub>N/GaN heterostructures ( $x = 0.25$ ) with spin-splitting energy 9.0 meV [1]. The large spin-splitting energy of the 2DEG was attributed to the anti-crossing of conduction bands [2]. The beating pattern was reproduced on another sample with a different alloy composition ( $x = 0.22$ ). By using a persistent photoconductivity [3], we have studied the spin-splitting pattern as a function of carrier concentration at different temperatures. We eliminated the possibility of magneto-intersubband scattering by temperature-dependent

SdH measurement, and also eliminated the possibility of inhomogeneity effect [4] due to the absence of negative magnetoresistance, which resulted from a weak anti-localization effect produced by the inhomogeneity effect. Based on the results, we proposed a p-wave-enhanced InGa<sub>x</sub>N/InAlN quantum well [3] for the application of spin-polarized field-effect transistor designed by Datta and Das [5].

[1] I. Lo, et al., Prys. Rev. B 65, 161306R, (2002) [Virtual Journal Nanoscale Science & Technology (4/29/2002)].

[2] I. Lo, et al. Appl. Phys. Lett. 88, 082108 (2006) [Virtual Journal Nanoscale Science & Technology (3/6/2006)].

[3] I. Lo, et al., Phys. Rev. B 74, 245325 (2006) [Virtual Journal Nanoscale Science & Technology (7/3/2007)].

[4] N. Thillozen, et al., Phys. Rev. B 73, 241311(R), (2006).

[5] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990).

11:15–11:30

## Nitride Semiconductor Nanostructures and Nanophotonics for Efficient Optoelectronics Devices

**Cheng-Yen Chen, Chi-Feng Huang, Yung-Sheng Chen, Wen-Yu Shiao, Dong-Ming Yeh, Kun-Ching Shen, Tsung-Yi Tang, Chih-Feng Lu, Yen-Cheng Lu, Cheng-Hung Lin, Shao-Ying Ting, Jeng-Jie Huang, Ming-Hsiu Chang, Tzu-Chi Liu, and Chih-Chung (C. C.) Yang\***

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**J. D. Albrecht**

*Air Force Research Laboratory, Sensors Directorate, Wright-Patterson Air Force Base, Ohio*

This presentation includes two parts. The first part is to discuss the growth of GaN nano-columns and their overgrowth for coalescence. This research represents a cooperation effort between US Air Force Research Laboratory (AFRL), Dayton, and National Taiwan University (NTU), Taipei. We will report the nano-material and optical analysis results of the GaN nano-columns grown with MBE at AFRL and the coalescence overgrowth samples with MOCVD at NTU. The growth of GaN nano-columns means to prepare threading dislocation-free GaN templates. The coalescence overgrowth means to implement flat GaN templates for optoelectronics and electronics device



fabrications. The second part is related to the study of nano-photonics, particularly related to the evaluation of the feasibility of using the coupling process of surface plasmon (SP) with InGaN/GaN quantum wells (QWs) for enhancing the quantum efficiency of such a light-emitting diode (LED). In such a device, a metal layer, such as silver, aluminum, and gold, of various morphologies is coated on the semiconductor surface close to the QWs. SP modes of various dispersion relations are generated at the interface between the semiconductor and the metal layer. The evanescent fields in the semiconductor extend into the QW layers such that the dipoles in the QWs can couple with the SP fields. Through the coupling process, the dipole energy can be transferred into the SP modes, similar to the process of stimulated emission. In this situation, if the SP modes can well phase-match with the emitted photons, radiation can occur through the SP coupling.

### 11:30–13:30 Buffet Lunch

### 11:45–13:30 Poster Set-Up

*You are encouraged to leave your poster up as long as you would like, as these will be available for viewing in a common area throughout the meeting. However, please take down your poster no later than 15:00 on Friday, February 9.*

### 13:30–14:45 Session 3: Electro-Optical properties of Nanostructures

*Dr. Bill Mitchel (AFRL Materials and Manufacturing Directorate), Chair*

13:30–13:45

### High Efficiency and Long Life Photovoltaic Research for Space Applications

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Polymer photovoltaic device is favored over wafer based semiconductor photovoltaic device due to its light weight and flexible behavior. However, the polymer photovoltaic device usually has shortcomings in low efficiency and short life. We are proposing to make high efficiency and long life photovoltaic devices from aromatic polymer-oxide nanoparticle hybrid material

containing ordered nanostructure for space applications. We have established time resolved photoluminescence spectroscopy to measure exciton life time and time of flight photoluminescence spectroscopy to measure charge carrier mobility. By inclusion CdSe nanoparticles into MEHPPV conducting polymer in the hybrid solar cell increases the ordering in polymer. The absorption spectrum was red shifted for hybrid system as compared with neat polymer. The hybrid system also exhibits an order increase in power efficiency (2006 *Nanotechnology* 17, 1260). The exciton life time of hybrid material can be decreased to less than half of the neat polymer by inclusion low cost and nontoxic TiO<sub>2</sub> nanorod into MEHPPV conducting polymer (2006 *Nanotechnology*, 17, 5781-5785). The TiO<sub>2</sub> nanorod-MEHPPV solar cell has been fabricated. The efficiency of cell can be increased by 2.5 times by inserting a TiO<sub>2</sub> nanorod electron transport layer between the hybrid active layer and metal electrode (2006 *Nanotechnology* 17, 5387-5392). The charge carrier mobility of P3HT polymer can be increased at least an order by blending TiO<sub>2</sub> nanorods into P3HT. The carrier mobility can be further increased using column structured ZnO electron transport layer infiltrated with the TiO<sub>2</sub>-P3HT hybrid. Environmentally friendly, red absorbing and water soluble polythiophene (poly [2- (3-thienyl) ethyloxy-4-butyl sulfonate]) (PTEBS) and spectrum tunable homogeneous TiO<sub>2</sub>-P3HT hybrid have been synthesized for high efficiency solar cell.

13:45–14:00

### Shell/Core Nanoparticles for Optoelectronic Applications

**T. Randall Lee**

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The optical absorbances of monometallic nanoparticles with core-shell geometries can be tuned from the visible to near infrared by varying the core size and shell thickness in a systematic fashion. These nanoparticles, called “nanoshells”, typically consist of a dielectric silica core ( $\geq 100$  nm diameter) surrounded by a gold shell ( $\leq 30$  nm thick). As such, they have been targeted for use in a variety of applications, including Raman-based imaging, cancer therapy, and optical shielding. Here, we wish to report the preparation and characterization of discrete metallic silver core particles that are coated with a thin metallic gold shell. At selected dimensions, these composite particles absorb strongly in the visible and/or near infrared spectral regions. Importantly, they can be prepared with substantially greater ease and markedly smaller sizes than the previous generation gold-coated silica nanoshell particles.

14:00–14:15

## Novel carbon-Al complex nanolayer in efficient organic/polymer light-emitting diodes

Tzung-Fang Guo,<sup>\*</sup> † Fuh-Shun Yang,<sup>†</sup>  
Zen-Jay Tsai,<sup>†</sup> and Ten-Chin Wen<sup>‡</sup>

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Incorporating a thin organic-oxide functionalized nanolayer with Al yields a composite cathode structure for the fabrication of high-performance organic/polymer light-emitting diodes (O/PLEDs). The electroluminescence (EL) efficiency of phenyl-substituted poly(para-phenylene vinylene) copolymer-based PLEDs with an organic oxide/Al composite cathode, reaches 12.20 cd/A, which is markedly higher than those, 5.26 cd/A and 0.11 cd/A, of devices with Ca/Al and Al cathodes, respectively. The improved device performance is due to the instant formation of a specific carbon-Al complex nanolayer at the cathode interface during the deposition of Al. As characterized through the depth-profile measurement of X-ray photoelectron spectroscopy, an Al-C interlayer is found at the cathode interface, which works as a medium enabling the efficient injection of electrons through the Al electrode and eliminating the metal-induced quenching sites of luminescence in the EL layer near the recombination region.

14:15–14:30

## Plasma-like negative capacitance in nano-colloids

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Recently, there has been a rapid increase in the number of reports describing negative capacitance (NC) in various nanostructures. In order to explore the conditions and possible mechanisms responsible for such observations we have investigated several nano-colloids which exhibit NC. The response of these systems is linear over a broad range of conditions. The low frequency dispersions of both the resistance and capacitance are consistent

with the free-carrier plasma model. Furthermore, we observe that the phenomenon is sensitive to the surface/volume ratio of the nanoparticles and the possible interfacial water. The possible mechanisms, ranging from a negative dielectric constant to nonlinear resistance with relaxation, are explored. It appears that plasma-like excitations and a new energy storage mechanism are needed to interpret the data.

14:30–14:45

## Controlled Zn/ZnO transformation and doped ZnO nanostructures with tunable optical properties

Wei-Yu Chen<sup>1</sup>, Ruey-Chi Wang<sup>2</sup>,  
and Chuan-Pu Liu<sup>1, 3,\*</sup>

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Diverse Zn, Zn/ZnO polyhedral particles and doped ZnO single-crystalline nanostructures with tunable optical properties were synthesized on Si substrates via a combination of thermal chemical vapor deposition, oxidation annealing and alloying vapor deposition (AVD). The single-crystalline Zn polyhedral particles with size larger than several microns could be grown on the Si substrate where the possible epitaxial planes with Si(111) could be ZnO (0001), (01 $\bar{1}$ 0), and (01 $\bar{1}$ 1) facets. The novel phase transformation from Zn to ZnO were studied systematically by controlled annealing treatments, where the optical properties of the polyhedral particles and the interfaces between Si (111) and different Zn facets were studied by cathodoluminescence (CL) and high-resolution transmission electron microscopy (HRTEM), respectively. Besides, Al: ZnO and Co: ZnO 1D nanostructures with tunable doping concentration were synthesized by varying the alloying treatment temperature of AVD. HRTEM results show that the doped nanostructures are single-crystalline wurtzite structures growing along the <0001> direction. Room-temperature CL measurements show that both the ZnO polyhedral particles and doped ZnO nanostructures exhibit strong ultraviolet (UV) emissions with negligible green emissions. The UV emission of the ZnO polyhedral particles shifts to a lower energy from 3.38 to 3.33eV by increasing oxidation annealing temperature from 450 to 600°. However, the UV emission of the Al doped 1D nanostructures shift to a higher energy from 3.29 to 3.34eV due to Al incorporation.

**14:45–15:00 Break**

**15:00–16:15 Session 4: Biological Applications & Toxicity of Nanomaterials**

*Dr. Saber Hussain (AFRL Human Effectiveness Directorate), Chair*

**15:00–15:15**

**Toxicity Assessment of Engineered Nanomaterials: Human Health Impact of Future Nanotechnology**

**Saber Hussain, Andrew Wagner, Laura Braydich, Amanda Schrand, Craig Murdock, Christin Grabinski, and John Schlager**

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Nanomaterials, which are defined functionally as have a single dimensional feature within the 1 - 100 nanometers range, have been used to create materials that exhibit novel physicochemical properties and function imparted through this engineered, controlled feature size. Although nanomaterials are currently being widely used in advancing technology, there is a serious lack of information concerning the human health and environmental implications of manufactured nanomaterials. The assessment of nanoparticle potential adverse impact should be a fundamental requirement before large-scale production and technological implementation of novel materials. In view of their possible effect on human health our main focus is to define and/or classify nanoparticles based on the nature of their toxicity. The physicochemical properties of engineered nanomaterials, may induce a pro-oxidant environment in the cells that may imbalance cellular redox potential, thereby leading to adverse biological consequences, which includes initiation of inflammatory pathways. The results in various mammalian cell culture models indicated that ROS generation, mitochondrial dysfunction, morphological changes represent quantifiable toxicological responses for engineered nanomaterials. Further physicochemical properties of the nanomaterials, particularly size, dimension, crystallinity, chemical composition, charge, surface area, and surface energy determine the ROS generation capability under physiological condition. The main focus of this presentation will be to discuss basic research applied to discover biological interaction of nanomaterials and its relationship to potential human health concerns.

Cleared as AFRL-WS 06-0172.

**15:15–15:30**

**Biomedical Applications of Mesoporous Silica**

**Chung-Yuan Mou**

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Biocompatible nanomaterials with magnetic and luminescence properties have recently become an attractive research field. One of the rapidly developing research subjects is their biomedical applications, including magnetic resonance imaging (MRI) contrast agent, magnetic hyperthermia therapy, targeted drug delivery, biosensors and rapid biological separation.

Because mesoporous silicas possess unique properties of high surface area, large pore volume, uniform pore size, and low cytotoxicity, multifunctional mesoporous composites that display both magnetic and luminescent functionalities would be very useful in biomedical applications. We have developed a series of functional mesoporous materials such as gadolinium-incorporated nanosized mesoporous silica (Gd-MS), FITC attached mesoporous silica nanoparticles (FITC-MSNs), and multifunctional mesoporous silica nanoparticles (Mag-Dye@MSN). The magnetic property could be exploited in cell-sorting and MRI contrast agent. The fluorescence could be used in cell-image and mesopores could be used for drug deliver. We further investigate the applications of these nanoparticles in cell labeling (NIH3T3, stem cell, and cancer cell) and in vivo animal MR imaging. Cytotoxicity of the mesoporous silica materials was evaluated and little toxicity effect was found. These porous nanoparticles promise to have great potential in cell-tracking and drug delivery.

**15:30–15:45**

**Modular Designed Functional Nanoparticles for Clinical Theranostics**

**Dar-Bin Shieh<sup>1</sup>, Cheng-Shen Yeh<sup>2</sup>, Yonhua Tzeng<sup>3,4</sup>**

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Cancer cells express certain proteins on their surface different from their normal counterpart, and have been an important field of study for molecular characterization and targeted therapy. Nano-materials usually display physical and chemical properties different from their bulk state and can be applied for biomedical applications of disease diagnosis and therapy, or even better, the theranostics approach. Combination of the two technology platform enabled improved molecular imaging and targeted delivery that may lead to better evidence based therapy and devoid of systemic side effects. We have integrated biotechnology and nanotechnology to implement self-assembled modular designed functional nanoparticles and nanocapsules. The functionalized superparamagnetic nanoparticles showed both *in vitro* and *in vivo* targeting of orthotopic tumor animal models through an genetic engineered or synthetic fusion peptide containing the targeting moiety and a “nanotag” motif that form a strong specific affinity to nanoparticles with their counterpart surface chemistry. Oral cancer lesions were contrast out after intravenous injection of the particles under T2 MR imaging sequence. The iron oxide nanorods with porosity interior structure were then implemented for controlled targeted delivery of gene and drug as encapsulated by polyelectrolytes through LbL methodology. The magnetic nanorods were able to exhibit controlled or sustained release mode depending on the surface treatment. In summary, modular design of targeting moiety, functional module and the nanoparticle enabled efficient implementation of the functional nanoparticles toward clinical applications. The concept of theranostics and trackable drug delivery are expected to further improve clinical diagnosis and therapy of human diseases.

15:45–16:00

## **Nanoparticles in Biological System: from *in vitro* to *in vivo* Investigations**

**Chung-Shi Yang**

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There has been exciting progress on the development of novel nano-scaled materials that are of valuable and interesting applications. This raises increasing concerns over the compatibility and safety of these nano-scaled materials to the biological system or to the ecological system. One of the specific aims of nanoscience and nanotechnology projects at the National Health Research Institutes (NHRI), supported by the National Science and Naotechnology Program Office, is to conduct the interdisciplinary research on the possible safety issues of the

novel nanomaterials in biological entities. Currently, three major approaches are employed: (1) the establishment of a standard protocol of animals or cultured cells to the nanoparticle exposure; this protocol involves the setup of a exposure chamber that can mimic the exposure to airborne nanoparticles to living species; (2) the studies on the acute and chronic effects on *in vitro* cell cultures; the morphological and functional alteration upon the nanoparticle exposure will be observed, cell survival/apoptosis will be studied, and microarray-based toxicogenomic approach will be employed to profile the early safety of the nanoparticles. (3) studies on the acute and chronic effects on animals upon the exposure to nanoparticle; the biological fates including the adsorption distribution, metabolism and excretion, as well as the physiological condition and long-term health status will be examined and followed up. In this presentation, we will present the results of a systemic study of the nanoparticles exposure from the *in vitro* cell level to *in vivo* animals, employing quantum dots as an example.

16:00–16:15

## **Nanoscience and nanotechnology research at National Sun Yat-Sen University, Taiwan**

**N. J. Ho**

Center for Nanoscience and Nanotechnology and Department of Materials Science and Optoelectronics, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China

National Sun Yat-Sen University has engaged in an international collaboration initiative that would bring excellent groups together to work on relevant subjects of modern time. This covers a wide spectrum of academic discipline and the Center of Nanoscience and Naotechnology is among the most active in this joint effort pursuit. For example, the collaborations between the University of Houston's Texas Center for Superconductivity, which is funded by the SPRING program, and Paul Drude Institute for Solid State Electronics in Berlin all have proved to be very productive and effective in both scientific discovery and education of students. In this talk, I will use examples in nanofabrications of nanostructures and nano-scale characterizations to give a general overview of all endeavors taking place in the campus and how such international efforts have worked.

**16:30–18:00 Poster Session I**

I-1

**Nanoindentation of Single Crystal Gold Nanowires****D. Cakiroglu<sup>1</sup>, D. Coker<sup>\*1</sup>, B. Ozturk<sup>2</sup>, and B. Flanders<sup>2</sup>**<sup>1</sup>School of Mechanical and Aerospace Engineering, <sup>2</sup>Department of Physics Oklahoma State University, Stillwater, OK 74078  
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Measurement of the mechanical properties of nanowires by indentation is difficult due to the influence of the curvature and substrate. The most widely used method to measure these properties is the Oliver-Pharr method (OP). However, Nix's group (2006) showed that OP method overestimates the contact area and contact depth in soft materials, thus underestimating the hardness and Young's modulus which makes use of these geometry parameters. Joslin-Oliver (JO) method can give better approximation for the hardness of soft materials because this method uses the term  $P/S^2$  which does not depend on the indentation depth and contact area. JO has been shown to be accurate for the thin film systems having similar moduli such as gold film on a glass substrate. Single crystal gold nanowires of about 200 nm height, 1300 nm width and 200  $\mu$ m length were fabricated between two gold electrodes on a glass substrate using ENFilADIng (Electrochemical Nano-Filament Assembly with Directed Interfacing). The load-displacement behavior is measured using a nanoindenter which are analyzed using the JO and the OP method to obtain the hardness and modulus. The hardness values and modulus values are presented for single crystal gold nanowires using these two methods.

I-2

**Sensitive measurement of deep hole traps in conjugated polymers****Rodrigo E. Palacios, Wei-Shun Chang, John K. Grey, Fu-Ren F. Fan, Allen J. Bard<sup>\*</sup>, and Paul F. Barbara<sup>\*</sup>**Center for Nano and Molecular Science and Technology, University of Texas, Austin, TX  
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The recently developed single molecule spectroelectrochemistry (SMS-EC) technique was used to investigate deep hole-traps in the conjugated polymer poly(2,5-bis(2'-ethyl-hexyl)-1,4-phenylenevinylene) BEH-PPV at an interface with an indium tin oxide (ITO) electrode. Hole-traps in organic semiconductor materials are known to play an important role in charge injection and transport in organic electronic devices. In this report we demonstrate that the average hole-trap concentration is negligible

(<  $10^{11}$  traps/cm<sup>2</sup>) in a pristine polymer/electrode interface, corresponding to less than one trap per  $\sim 10^4$  oxidizable states. In contrast, under highly oxidizing conditions, "transient" hole-traps were observed. Under re-reducing conditions, the transient hole-traps are converted back to non-trap states over a broad distribution of time scales. Additionally, the rate of converting hole-traps to non-trap states is substantially accelerated by optical excitation. The results give further insight into the chemical nature of hole-traps in organic semiconductor materials.

I-3

**Energy Transfer and Selective Hole Injection in Blend Conjugated Polymers****Wei-Shun Chang, Ya-Lan Chang, Fu-Ren F.****Fan, Allen J. Bard<sup>\*</sup>, and Paul F. Barbara<sup>\*</sup>**

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Energy transfer and selective hole injection in polymer nanoparticles composing of F8BT (donor) doped with single polymer chain BEH-PPV (acceptor) was studied with the new electrochemical single molecule spectroscopy (EC-SMS) technique. At potential  $\sim 0.9$ V only BEH-PPV became oxidized (selectively creating holes on BEH-PPV) allowing us to explore the mechanism of forming deep trap. The relative energy transfer efficiencies (calculated from the intensity ratio of BEH-PPV and blend nanoparticles) were found as change linearly with the amount of the acceptor present, i.e.  $0.13 \pm 0.11$  and  $0.66 \pm 0.20$  for 1% and 6% blend nanoparticle, respectively. Assuming an average nanoparticle diameter of 25nm, we estimated a forster radius of 6nm. At 1% of BEH-PPV in nanoparticles, the acceptor component showed fluorescence intermittency suggesting that single chain doping levels were achieved at this concentration. The ensemble fluorescence intensity of 1% blend nanoparticle was quenched  $\sim 15\%$  with applying triangular bias of 0.9V consistent with the fraction of fluorescence for BEH-PPV in 1% blend nanoparticle, while very little fluorescence quenched for pure F8BT aggregates. This result suggests that the potential driven oxidation of BEH-PPV only quenched the fluorescence from BEH-PPV. No further significant intensity quench under a pulse bias of 0.9V with duration of 5s suggests that the holes on BEH-PPV chains are localized and does not diffuse into the F8BT polymers. A symmetric and reversible intensity modulation of 1% blend nanoparticles with applied pulse bias of 0.9V suggests that the holes injection into single BEH-PPV chain does not form a deep trap. This result is consistent with the proposed mechanism

that multiple chains are required to form a strong acid to be deprotonated, which is the source of deep trap.

I-4

### 3D Nano-photonic Crystal structures for Laser Beam Switching and Steering

Jiaqi Chen<sup>a)</sup>, Wei Jiang<sup>b)</sup>, Xiaonan Chen<sup>a)</sup>, Li Wang<sup>a)</sup>, Sasa Zhang<sup>a)</sup> and Ray T.Chen<sup>\*</sup>

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Photonic crystal based superprism offers a new way to design new optical components for beam steering and DWDM application. 3D photonic crystals are especially attractive as they could offer more control of the light beam based on the needs. A polygonal prism based holographic fabrication method has been demonstrated for a three-dimensional face-centered-cubic (FCC)-type submicron polymer photonic crystal using SU8 as the photo-sensitive material. Therefore antivibration equipment and complicated optical alignment system are not needed and the requirement for the coherence of the laser source is relaxed compared with the traditional holographic setup. By changing the top-cut prism structure, the polarization of the laser beam, the exposure and development conditions we can achieve different kinds of triclinic or orthorhombic photonic crystals on demand. Special fabrication treatments have been introduced to ensure the survivability of the fabricated large area (cm<sup>2</sup>) nano-structures. Scanning electron microscopy and diffraction results proved the good uniformity of the fabricated structures. With the proper design of the refraction prism we have achieved a partial bandgap for S+C band (1460-1565nm) in the [111] direction. The transmission and reflection spectra obtained by Fourier transform infrared spectroscopy (FTIR) are in good agreement with simulated band structure. The superprism effects around 1550nm wavelength for the fabricated 3D polymer photonic crystal have been theoretically calculated and such effects can be used for beam steering purpose.

I-5

### Self-Assembled Monolayers Generated from Unsymmetrical Partially Fluorinated Spiroalkanedithiols

Pawilai Chinwangso and T. Randall Lee\*

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The structural and interfacial properties of self-assembled monolayers (SAMs) generated from the adsorption of the chelating dithiol (CH<sub>3</sub>(CH<sub>2</sub>)<sub>7</sub>C[(CH<sub>2</sub>)<sub>8</sub>(CF<sub>2</sub>)<sub>7</sub>CF<sub>3</sub>][CH<sub>2</sub>SH]<sub>2</sub>) onto the surface of gold were investigated. These new SAMs were characterized by ellipsometry, contact angle goniometry, polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS), and X-ray photoelectron spectroscopy (XPS). These data were compared to those obtained from SAMs generated from *n*-octadecanethiol (C18SH, CH<sub>3</sub>(CH<sub>2</sub>)<sub>17</sub>SH) and the semifluorinated thiol (F8H10SH, CF<sub>3</sub>(CF<sub>2</sub>)<sub>7</sub>(CH<sub>2</sub>)<sub>10</sub>SH). The latter two monothiols possess terminal chains with chemical compositions analogous to those found in the new chelating dithiol.

I-6

### Synthesis, Optical and Fluorescence Studies of Gold nanoparticle Polymer Composites with Carbazole Terminated Dendrons.

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I-7

### Structural and Mechanical Properties of Graphene Oxide Paper

Dmitriy A. Dikin,<sup>†</sup> Sasha Stankovich,<sup>†</sup> Eric J. Zimney,<sup>†</sup> Geoffrey H. B. Dommett,<sup>†</sup> SonBinh T. Nguyen,<sup>‡</sup> and Rodney S. Ruoff<sup>†</sup>

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Free standing membranes (graphene oxide paper) were produced by exfoliation of graphite oxide in water to individual 'graphene

oxide' sheets (as a colloidal suspension) followed by their re-assembly by vacuum filtration. Study of the structure and morphology of the graphene oxide paper revealed that it is composed of highly packed and ordered layers of graphene oxide sheets separated by intercalated and H-bonded water molecules. Measurements of the mechanical response under tensile load revealed elastic deformation for small strain, followed by plastic deformation again for a relatively small region of strain, and then fracture without pullout of individual sheets or multi-layer stacks. Graphene oxide paper possesses high modulus values of about 40 GPa and strength values around 130 MPa, each much higher than modulus or strength values for either bucky-paper or commercial Grafoil. The experimental results support the conclusions of very effective load distribution and good binding between the graphene oxide sheets in which the self-regulated amount of interlayer (intercalated) water plays a central role.

Support from NASA and the NSF is appreciated. Both grants end in August 2007.

I-8

## Particle size influence on the magnetic properties of $\text{HoMnO}_3$ multiferroic

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The hexagonal, nonperovskite  $\text{HoMnO}_3$  oxide, containing a triangular arrangement of  $\text{Mn}^{3+}$ , has been prepared with nano- and micro-size particles using the novel self-sustaining one-step process, named Carbon Combustion Synthesis of Oxides. X-ray diffraction and electron probe microanalysis of as-synthesized powders show that essentially complete conversion to single-phase products was accomplished during the synthesis.  $\text{HoMnO}_3$  single crystals are well known as multiferroic, where the Ho-O displacements give rise to a ferroelectric moment ( $T_C = 875$  K), the  $\text{Mn}^{3+}$  moments order at Néel temperature  $T_N = 72$  K,  $\text{Mn}^{3+}$ -spin reorientation transitions occur at  $T_{sp} = 34$  K, magnetic  $\text{Ho}^{3+}$  orders at  $T_{Ho} \sim 5.2$  K, and the order parameters are naturally coupled through the Ho-Mn exchange and anisotropy interactions. We have investigated the influence of nano/micro size particles on the magnetic behavior in combustion-synthesized  $\text{HoMnO}_3$  materials in comparison with a polycrystalline samples crushed from a  $\text{HoMnO}_3$  single crystal. Below 5 K we have observed magnetic hysteresis phenomena. Magnetic coercive field, as well as remnant magnetic moment, increases with diminishing

particle size. We assume that the hysteresis behavior in the polycrystalline particles occurs due to a single-domain state, in which the only mechanism for the magnetization reversal is the rotation of the particles magnetic moment. This rotation requires more energy against the anisotropy forces and higher fields are required to reverse the magnetization.

I-9

## Nonlinear elastic behavior of graphene sheets and single-wall carbon nanotubes

Jun Zhou and Rui Huang

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A continuum analysis incorporating interatomic potentials is conducted in order to understand the nonlinear behavior of carbon nanotubes (CNTs) under finite deformation. The classical Cauchy-Born rule provides a bridge linking between atomic interactions and macroscopic stress-strain behavior. However, since the atomic structure of CNTs is not centrosymmetric, it is necessary to modify the Cauchy-Born rule to account for internal relaxation of atoms, which renders locally inhomogeneous deformation at the atomic scale under a macroscopically homogeneous strain. By molecular mechanics simulations, we show that, for a unit cell of planar graphene sheet, the atomic positions shift from those predicted by homogeneous deformation except for the case with equi-biaxial strain. A linear relationship is obtained for the atomic shift under relatively small strains, which becomes nonlinear under larger strains. By incorporating the internal relaxation into the Cauchy-Born rule, we show that the in-plane stress-strain behavior of a graphene sheet becomes nonlinear and anisotropic under finite deformation. In particular, a coupling between normal and shear deformation is predicted along the directions corresponding to chiral CNTs, in agreement with previously reported stretch-induced torsion in single-wall CNTs.



I-10

## **An Analysis of SAMs on Gold Derived from $\text{CH}_3\text{CF}_2(\text{CH}_2)_n\text{SH}$ Provides Insight into the Influence of Fluorine Substitution on Chain Conformation**

**Andrew C. Jamison, David Barriet and T. Randall Lee\***

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Self-assembled monolayers (SAMs) prepared from a series of alkanethiols in which the terminal methylene group was selectively fluorinated ( $\text{CH}_3\text{CF}_2(\text{CH}_2)_n\text{SH}$ , where  $n = 11-16$ ) were analyzed using *ab initio* calculations employing the 6-31G\* basis set at the level of restricted Hartree-Fock (RHF). Additional structural information was gathered using optical ellipsometry, contact angle goniometry, transmission infrared spectroscopy, and polarization modulation infrared reflection absorption spectrometry (PM-IRRAS). The PM-IRRAS spectra show that the presence of the  $\text{CF}_2$  unit fails to disrupt the formation of well-ordered SAMs in the adsorbates having longer chains; these data also provide evidence that the longer chain SAMs are more crystalline in their packing structure than those having shorter chains. There are, however, indications that the SAMs having odd-numbered chain lengths fail to exhibit the all-*trans* alignment that is expected for such monolayers. This presentation examines the evidence that the odd-numbered chains of this series are skewed from their anticipated alignment. Moreover, our analysis shows that these deviations from the anti conformation at the end of the chain can occur without disrupting the ordered structure of the SAM.

I-11

## **Alternate Ultrathin Films of CdSe Nanoparticles and Conjugated Polymers; Band Gap Design for Solar Cells and Memory Devices.**

**Jayarathne, L. C.; Park, Y. Baba, A.; Fulghum, T. M.; G. Jiang.; Advincula, R.**

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Electrostatic layer by layer self assembly was incorporated to deposit nanocomposite thin films of a p-type organic semiconductor, Emeraldine base of polyaniline (EB-PANI) and an n-type inorganic semiconductor, thiol coated CdSe nanoparticles (CdSe-T) on ITO coated glass substrates. In-situ Surface Plasmon Resonance Spectroscopy (SPS) was used

to obtain the correct concentrations of EB-PANI and CdSe-T solutions, in order to achieve nanoscale control of hybrid thin films. The dielectric constant and thickness of thin films were determined using SPS and Ellipsometry respectively. UV-vis spectroscopy and Cyclic Voltammetry of as deposited films were investigated as a function of number of bilayers and the appropriate band gap and the number of bilayers were proposed to construct solar cells and memory devices.

I-12

## **Covalent Immobilization of Patterned Monolayers of Magnetic Nanoparticles on Hydrogen-Terminated Silicon.**

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In this study,  $\omega$ -alkenyl-1-carboxylic acids was synthesized as a surfactant, which was used in the direct preparation of magnetic iron oxide ( $\text{MnFe}_2\text{O}_4$ ) nanoparticles with the surfactant subsequently bound to a silicon(100) surface. The magnetite nanoparticles terminated with the  $\alpha$ -alkenyl moieties was prepared using a one-pot reaction at high temperature without the need of ligand exchange. This process led to the creation of monodisperse magnetite nanoparticles. Transmission electron microscopy and X-ray diffraction measurement were used to characterize the morphology and structure of the nanoparticles. The nanoparticles were deposited as prepared onto a hydrogen-terminated silicon(100) wafer, and covalently anchored to the surface by UV irradiation at 365 nm. Analysis was conducted by AFM, SEM, SQUID and XPS with UV treatment, confirming that the UV treatment led to covalent immobilization of the nanoparticles on the silicon surface.

I-13

## **Fabrication and Mechanical Characterization of Silicon Nanolines**

**Bin Li<sup>a,\*</sup>, Min K. Kang<sup>b</sup>, Kuan Lu<sup>a</sup>, Rui Huang<sup>b</sup>, Paul S. Ho<sup>a</sup>, Richard A. Allen<sup>c</sup>, Michael W. Cresswell<sup>c</sup>**

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With continuing scaling of device dimension, fabrication of nanoscale structures and characterization of their mechanical properties pose significant challenges for future development of ultra large-scale integrated (ULSI) circuits. In particular, silicon-based nanostructures form essential building blocks for microelectromechanical systems (MEMS) and play an important role in controlling the functionality and reliability of devices. In this study, we demonstrate the feasibility of a method to fabricate nanoscale Si lines using an anisotropic wet etching process. The silicon nanolines have straight and atomically flat sidewalls, almost perfectly rectangular cross sections and highly uniform linewidth at the nanometer scale. Nanolines with a height-width aspect ratio ranging from 1 to 10 have been successfully fabricated. An atomic force microscope (AFM) based nanoindentation system was employed to investigate the scaling effect on mechanical properties of the silicon nanolines. The indentation force-displacement curves were determined for a set of Si lines with line widths ranging from 70 to 500 nm. Interestingly, after the initial elastic response, a large displacement burst was observed for nearly all the lines. After unloading, for silicon lines of 73nm wide no residual deformation was observed, suggesting an elastic deformation mechanism. We attribute the observed displacement burst to buckling of the nanolines as a bifurcation to the initial elastic deformation under indentation. A finite element model is being developed to predict the critical load for buckling and will be used to analyze the observed buckling behavior. Finally the scaling effects on elastic modulus and strength of the silicon nanolines will be discussed.

I-14

## **A TiO<sub>2</sub>-anatase implanted nano-layer on glass curtain to improve indoor air quality**

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A comfortable space is particularly emphasized in modern architecture, while a moderate introduction of natural sunlight and free air is anticipated. This work is to improve indoor air quality by reducing ambient air temperature and cleaning indoor airflow, which aims to make life more comfortable and simultaneously to achieve energy saving more efficient. By upholding the degree of sunlight transmission, the inner glass surface is a TiO<sub>2</sub>-anatase implanted nano-layer that is photo-catalytic, peeling-resistant and high in contact surface area. The ultra-thin nano-layer is competent to absorb particular wavelengths from the transmitted sunlight and promote the photo-catalytic reactivities such as the decomposition of organic species and odors, the control of bacterial growth. It is therefore functioned to clean a major part of the indoor airflow. In addition, the pathway of the airflow can be installed with air filters that are purposely implanted with silver ions. The silver ion-implanted filters are also applicable to kill bacteria during the night or a cloudy day.

I-15

## **A new model developed to evaluate the contact parameters arising during the nano-indentation tests with different loading/unloading rates**

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A new mechanical model is developed in the present study for hard materials to investigate the behavior arising during the loading/unloading process of an indentation test. Two governing differential equations are derived for the depth of the indenter tip ( $h_i$ ) and the depth formed at the separation point ( $h_s$ ) expressed in a power form. The exponent value of  $h_i$  in either the loading process or unloading process is considered to be a variable as a function of the indentation depth in the governing differential

equation. The exponent value of  $h_s^*$  is proven to be the same value as that of  $h_i^*$ . All spring and damping coefficients shown in these governing differential equations are determined by the real-coded genetic algorithm. With the aids of experimental results of  $h_i$  shown at large and small indentation depths, the  $h_i^*$  and  $h_s^*$  solutions are obtained. The asymptotic solutions of  $h_i^*$  and  $h_s^*$  at various indentation depths can thus be determined, and the real contact area at any indentation depth can be calculated if  $h_s^*$  is available. Quartz was used as the example of hard materials, and the contact area predicted by the present model is quite close to the solution predicted by the area function of Oliver and Pharr [1]. Under a constant maximum load, the contact projected area is slightly increased by decreasing the loading/unloading rate. The phase lag behavior demonstrated in the indentation test at two different loading/unloading rates was investigated, and it is enhanced by increasing the loading/unloading rate.

I-16

## Quantitative Nano-friction Study of Vertically Aligned Multi-Walled Carbon Nanotube Arrays

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Sliding friction properties of vertically aligned multi-walled carbon nanotube (VAMWNT) arrays have been investigated in current study. The VAMWNT arrays have been obtained on an anodic aluminum oxide (AAO) template by chemical vapor deposition at 650°C. Friction force was measured in air by a modified lateral force microscopy (LFM) tip with 15 µm diameter borosilicate sphere attached to the end of the regular LFM tip. Direct friction force calibration at nano scale was carefully carried out by using a novel diamagnetic levitation calibrator system. A reverse stick-slip behavior was observed and investigated by energy optimization analysis. The effects of protruded lengths (0, 30, 100, 750 nm) of these VAMWNT arrays and different interfaces were studied systematically. It was found the resulting friction forces increases with increasing protruded length. Also, Aluminum coated cantilever-bead assembly results higher friction forces in all samples studied.

I-17

## Nano-ripple structure formation on Silicon surface by gas cluster ion beam fabrication and its applications to III-nitride nanorods fabrication

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Gas cluster ion beam (GCIB) have been used to fabricate nano-ripple structures on Si substrates. In this work, using  $(Ar)_n^+$  clusters at 30 kV acceleration, where  $n \approx 3,000$ , we have observed nano-ripple formations on the silicon surface after GCIB bombardment. The wavelength, amplitude and the dimensions of the ripples are studied in an effort to characterize the morphology as a function of cluster beam's angle of incidence, crystallographic orientations of the substrate, and the ion dosages. The underlying physics of ripple formation will be conjectured and the applications of nanostructures fabrication on rippled (111)-Si substrates in producing nanorods of III-nitrides, such as GaN, InGaN, and InAlN, will be presented.

18:00–20:00 Dinner

20:00–21:30 Poster Session II

II-1

## Ultraviolet photodetectors with ZnO nanowires prepared on ZnO:Ga/glass templates

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Vertically well-aligned ZnO nanowire ultraviolet (UV) photodetectors were fabricated by spin-on-glass technology on ZnO:Ga/glass templates. With 2 V applied bias, it was found

that dark current density of the fabricated device was only  $3.8 \times 10^{-9}$  A/cm<sup>2</sup>. It was also found that UV-to-visible rejection ratio and quantum efficiency of the fabricated ZnO nanowire photodetectors were more than 1000 and 12.6%, respectively. It was also found that noise equivalent power and normalized detectivity of the ZnO nanowire photodetector were  $5.73 \times 10^{-11}$  W and  $6.17 \times 10^9$  cmHz<sup>0.5</sup>W<sup>-1</sup>, respectively.

## II-2

### **Synthesis of Tert-Butyl-Terminated Alkanethiols for the Generation of Sterically Crowded Self-Assembled Monolayers (SAMs) on Gold**

**Justin Moore**

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## II-3

### **Formation of silver nanoparticles in silicon by metal vapor vacuum arc ion implantation**

**Q.Y. Chen<sup>1,3</sup>, H.W. Seo<sup>2</sup>, I.A. Rusakova<sup>1</sup>, L.W. Tu<sup>3</sup>, Y.L. Cheng<sup>3</sup>, Z. H. Zhang<sup>1</sup>, X. M. Wang<sup>1</sup>, J.R. Liu<sup>1</sup>, O. Lozano<sup>1</sup>, and W. K. Chu<sup>1</sup>**

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In this work, Ag nanoparticles embedded in Si matrices were fabricated by ion-implantation of Ag atoms into Si substrates using a high beam-current metal vapor vacuum arc (MEVVA) ion source. Nano-precipitations of the Ag phase takes place when an Ag-Si solid solution is oversaturated. The experiments were conducted at an acceleration voltage of 50 keV and ion flux of  $\sim 5 \mu\text{A}/\text{cm}^2$ . The Ag-ions were extracted from the MEVVA ion source in three main charge states, with the average charge of Ag<sup>+n</sup> being  $\langle n \rangle \approx 2$ . The implantation dosage was  $1 \times 10^{17} / \text{cm}^2$ . The sizes of the nanoparticles are uniformly distributed, about 6 nm on the upper 55 nm and 2 nm near the bottom 5 nm of the overall 60 nm layer amorphized by the ion bombardments. Various attempts of post-implantation treatments were made to recrystallize the amorphous silicon layer through solid phase epitaxial growth. Optical and electrical characterizations of the nanocomposite system will be presented.

## II-4

### **Electroluminescent Properties of Poly(phenylenevinylene) (PPV) and Copolymer: Synthesis and Characterization of poly(2,5-didecyl-1,4 phenylenevinylene), poly(2,5-didecyloxy-1,4 phenylenevinylene), and their copolymer**

**Sairoong Saowsupa, and T. Randall Lee**

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In this study, poly(2,5-didecyl-1,4-phenylenevinylene), poly(2,5-didecyloxy-1,4-phenylenevinylene), and their copolymer were synthesized via the Horner-Emmons route. The optimum conditions for preparing all polymers were studied at various temperature, 50, 80, and 100 °C, using the same solvent system. The structure of the polymers was characterized by NMR spectroscopy, gel permeation chromatography (GPC), UV-vis, fluorescence, photoluminescence, and electroluminescence spectroscopy. Tests were conducted to determine the molecular weight and polydispersity of each temperature that generate the polymer. UV-vis spectra showed a slightly bathochromic shift when the polymers were produced at a higher temperature. The findings indicate that the Horner-Emmons route produced poly(2,5-didecyl-1,4-phenylenevinylene), poly(2,5-didecyloxy-1,4-phenylenevinylene), and their copolymer with high molecular weight, low polydispersity, and high yield. The study of optical properties and lifetime of the OLEDs based on these polymers, and comparing the result will be obtained.

## II-5

### **GaN nanorod arrays on Si self-implanted (111) Si-substrates**

**H.W. Seo<sup>1,2</sup>, N. Badi<sup>1</sup>, Q.Y. Chen<sup>1,3</sup>, L.W. Tu<sup>3</sup>, Y.T. Lin<sup>3</sup>, Y.L. Cheng<sup>3</sup>, X.M. Wang<sup>1</sup>, J.R. Liu<sup>1</sup>, O. Lozano<sup>1</sup>, and W.K. Chu<sup>1</sup>**

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We have successfully fabricated the array pattern of epitaxial GaN nanorods by self-implantation on Si substrates. The ion



bombardments prior to deposition induce changes of surface morphology of Si substrate and thus, in the film growth, results in the formation of capillary tubes, which are the valleys surrounded by islands. This is attributed to the nanocapillary condensation of Ga droplets that serve as a medium to the vapor-liquid-solid growth of nanorods out of its supporting matrix. The morphology of substrate is closely related to the parameters during the implantation process which determine the size and density of nanorods.

## II-6

### **Nanoscale Piezoelectricity and the Possibility of Apparently Piezoelectric Composites without using Piezoelectric Materials**

**P. Sharma**

*Department of Mechanical Engineering, University of Houston, Houston, TX, 77204, U.S.A*

In a piezoelectric material an applied *uniform* strain can induce an electric polarization (or vice-versa). Crystallographic considerations restrict this technologically important property to non-centrosymmetric systems. It has been shown both mathematically and physically, that a *non-uniform strain* can potentially break the inversion symmetry and induce polarization in non-piezoelectric materials. The coupling between strain gradients and polarization; and strain and polarization gradients, is investigated in this work. Based on a field theoretic framework accounting for this phenomena, we (i) develop the fundamental solutions (Green's functions) for the governing equations (ii) solve the general embedded inclusion problem with explicit results for the spherical and cylindrical inclusion shape and, (iii) Illustrate using the simple examples how an apparently piezoelectric composite may be created without using constituent piezoelectric materials.

## II-7

### **Preparation, Characterization, and Stability of Gold Nanoparticles Coated with Mono-, Bis-, and Tris-Chelating Alkanethiols.**

**La-ongnuan Srisombat, Shishan Zhang, Joon-Seo Park and T. Randall Lee\***

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The formation of monolayer-protected nanoparticles (MPNs) generated by the adsorption of *n*-octadecanethiol, 2-hexadecylpropane-1,3-dithiol, 2-hexadecyl-2-methylpropane-1,3-dithiol, and 1,1,1-tris(mercaptomethyl)heptadecane onto gold nanoparticle cores is described. The MPNs were characterized by solubility, transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), and Fourier transform infrared spectroscopy (FT-IR). The gold nanoparticle cores were estimated to be 1-3 nm in diameter as evaluated by TEM. Analysis by FT-IR showed that MPNs functionalized with *n*-octadecanethiol possessed the highest chain crystallinity in both the solid-state and dispersed in solution; the self-assembled monolayers (SAMs) generated from the other three adsorbates were more liquid-like, but indistinguishable from each other. The rate of nanoparticle decomposition induced by cyanide ion was monitored by UV-vis spectroscopy. While MPNs functionalized with *n*-octadecanethiol showed the fastest rate of decomposition, those functionalized with 2-hexadecyl-2-methylpropane-1,3-dithiol were the most resistant to decomposition.

## II-8

### **Electropolymerization of Anionic Polycarbazole Precursor on Layer-by-layer Nanostructured films with Cationic Water-Soluble Sexithiophenes**

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## II-9

### **Graphite Oxide as a Source of Graphene Nanoplatelets Including for Nanocomposites**

**Sasha Stankovich, \* Dmitriy A. Dikin, \* Richard D. Piner, \* SonBinh T. Nguyen# and Rodney S. Ruoff\***

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Graphene sheets, the basic structural units of graphite, are predicted to have extraordinary mechanical, thermal and electrical properties. It is for this reason that carbon nanotubes, composed of rolled-up graphene sheets, have become attractive targets for numerous applications including as nano-fillers for composite materials. Production of carbon nanotubes is costly on

a large scale, however, severely hampering their utility. Graphite on the other hand is an inexpensive and abundant material that can serve as a viable source of graphene sheets provided it can be completely exfoliated.

Various routes for the synthesis of graphene-based composite materials will be presented. We first prepared graphene-based sheets via exfoliation of graphite oxide (GO). These resulting partially oxidized graphene sheets can then be chemically modified to fine tune their dispersion properties in organic solvents, their compatibility with various organic and inorganic matrices, and their electrical conductivity. For example, graphene oxide sheets produced by exfoliation of GO are derivatized by a treatment with organic isocyanates, which allows for their exfoliation in polar aprotic solvents. Following their incorporation into a polymer matrix such as polystyrene, the sheets are chemically reduced to prepare electrically conductive graphene/polystyrene composites with graphene sheets uniformly distributed within the matrix.

Support from NASA and the NSF is appreciated. Both grants end in August 2007.

## II-10

### Interdiffusion Behavior at the Interface between Deposits of Au Nanoparticles and Electronic Substrates

**Tzu-Hsuan Kao<sup>1</sup>, Jenn-Ming Song<sup>2</sup>,  
In-Gann Chen<sup>1</sup>, Teng-Yuan Dong<sup>3</sup>**

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Since nano-sized metallic powders exhibit a considerably reduced melting point compared to bulk materials, by using a proper deposition technique, for example, drop-on-demand ink jet printing, suspensions containing metallic nanoparticles (NPs) could be applied to manufacture desired conductive patterns after a low temperature thermal process. Thus, interconnects for microelectronic packaging could be prepared without the use of lithography-etching. This study investigated the interfacial behavior between thiol-stabilized Au NPs deposits and electronic substrates, Cu, Ni and Ag. After curing at a low temperature of 300°C, continuous Au films with acceptable adhesion strength could be obtained. Instead of sintering or agglomerating, curing at 300°C may result in an entire or partial melting of the deposited suspension because of the drastically reduced melting point of Au

NPs, measured to be 230 °C ~270°C, due to the nano-size effect. The elemental depth profiles and the chemical shifts of binding energy examined by an X-ray photoelectron spectroscopy (XPS) demonstrated that stoichiometric intermetallic phases existed at both the Au/Cu and Au/Ni interfaces, while a miscible solid solution layer was found to emerge at the interface between Au/Ag.

## II-11

### Nonvolatile Interfacial Resistive Switching on the Nanoscale

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A major driving force in nonvolatile memory research is the need to achieve ever decreasing device size scales. A possible candidate is the polarity-dependent field-induced resistive switch occurring at the interface between a metal electrode and an oxide material. The interfacial nanolayer created by the voltage pulses can be driven reversibly to either a nonvolatile low (on) or high (off) resistive state by a positive or a negative pulse. The switching in this nanolayer appears to be associated with modifications of the defect structures along percolative paths. Our results, therefore, indicate the possibility of locally switching individual nanoscale percolation paths, although the statistical limit based on the average interface resistivity may further restrict the device size. With better understanding of the switching mechanism and better interface control, nonvolatile resistive nanoscale memories are a possibility.

## II-12

### Nano-Nitrides and Applications

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Nitride nanorod structures are grown on Si(111) substrates by plasma-assisted molecular beam epitaxy. With the possible advantage of a less defective structure, potential applications are explored. In a proper growth parameter window with a buffer layer, sparse and well developed nanorods with a hexagonal shape are formed while under a growth condition without a buffer layer, high-density nanorods can be obtained. These nanorods are all aligned along a unidirection of crystallographic c-axis. Fundamental properties are characterized through a series of measurements and analyses including high-resolution transmission electron microscopy, field-emission scanning electron microscopy, photoluminescence, cathodoluminescence, micro-Raman spectroscopy, X-ray diffraction, energy dispersive spectrometer, etc. Double heterostructures of InGa<sub>N</sub>/Ga<sub>N</sub> are grown under various growth conditions with a basic p/n junction structure in the nanorods. Ni/Au contacts on p-GaN are fabricated and electroluminescence is performed. Colors in visible range from red to purple are seen.

#### II-13

### Recent progress on growth of GaN/AlGa<sub>N</sub> quantum confined structures for THz quantum cascade laser

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The quantum-cascade laser (QCL) has, since its first realization, demonstrated an impressive and rapid development, extending the emission wavelengths from mid-infrared to terahertz spectral range. However, QCLs based on GaAs/AlGaAs and AlInAs/GaInAs are not capable of emitting in the energy range around the LO-phonon energies, leaving a gap in the spectral scale between 30 and 40  $\mu\text{m}$ . The QCL based on AlGa<sub>N</sub>/Ga<sub>N</sub> material has been reported as a promising candidate for generating emission in this wavelength range. One of the key technical issues for realization of AlGa<sub>N</sub>/Ga<sub>N</sub> based QCL is the growth of high quality Ga<sub>N</sub> structures suitable for fabrication of QCLs. In particular the good surface morphology, Al compositional accuracy, and precise thickness control of the quantum well of the grown structure are very important factors for the QCL. In this report we present the recent progress on the growth of AlGa<sub>N</sub>/Ga<sub>N</sub> quantum confined structure using metal organic chemical vapor

deposition (MOCVD). We have established growth conditions for obtaining good surface morphology Al<sub>x</sub>Ga<sub>1-x</sub>N epitaxial layer with Al composition ranging from  $0 < x < 1.0$ . A 60-period quantum cascade Ga<sub>N</sub>/AlGa<sub>N</sub> structure suitable for serving as the active region of THz QCL was grown and analyzed. The grown sample showed smooth surface morphology with sharp layer interfaces. The composition and thickness of each period of quantum well were estimated from the simulation of XRD satellite peaks and TEM measurements. Various phonon modes of the grown sample were also observed using Fourier transform infrared spectrometer. These preliminary results indicate the MOCVD should be a viable method for growth of AlGa<sub>N</sub>/Ga<sub>N</sub> based THz QCL structure.

#### II-14

### Graphene-silica Composite Thin Films

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#### II-15

### Silicon and metal silicide nanowires: Structure and energy decomposition analysis from first principles

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Successful synthesis of extremely thin, 1-10 nm diameter nanowires of silicon (Si) and metal-silicides (MeSi) has posed a compelling problem for theory: What energy factors contribute in the stability of such structures and what is the ground-state shape for the smallest diameters? We have developed a systematic approach which allows one to perform such evaluation. Notably, the best shape for SiNW appears to be pentagonal [1,2], for the diameters below 5-6 nm. For MeSiNW, we extend this energy-decomposition approach to the binary compounds and demonstrate its applicability by comparison with direct *ab initio* computations. First principle calculations using density functional theory and the gradient-corrected LSDA approximation have been performed to examine the structural, electronic, and elastic properties of Y and Ni encapsulated silicon clusters and (2,2) nanotubes. The total energy is decomposed into the bulk, surface, and edge contributions [2,3] and a simple equation proposed for

the cohesive energy  $E(n, m)$  of arbitrary wire as a function of its cross-section dimension  $n$  and  $m$ .

[1] Y. Lin, N. Gonzalez Szwacki, and B.I. Yakobson, chapter in: *Nanosilicon* (Elsevier, 2007).

[2] Y. Zhao and B. I. Yakobson, *Phys. Rev. Lett.* **91**, 035501-1 (2003).

[3] N. Gonzalez Szwacki and B.I. Yakobson, *Phys. Rev. B* **75**, 035406 (2007).

II-16

## **A Facile Method for Preventing the Aggregation of Large Gold Nanoparticles and the Fabrication of 2-D Arrays**

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Bidentate and tridentate surfactants were evaluated for their ability to stabilize large Au nanoparticles (>15 nm) in solution. Citrate-stabilized gold colloid (20-50 nm) treated with various of the multidentate surfactants were extracted from the aqueous phase and dispersed into toluene. The absence of gold colloid aggregation was confirmed visually and this observation was supported by dynamic light scattering (DLS) and UV-vis spectroscopy. The tridentate thiol (1,1,1-tris(mercaptomethyl)pentadecane) showed a superior ability in preventing large gold colloid from aggregation. For gold nanoparticles modified by these multidentate thiols, only bound thiolate ( $S_{2p3/2}$  binding energy of 162 eV) was detected by X-ray photoelectron spectroscopy (XPS). The large gold nanoparticles dispersed in nonpolar solvents are able to self-assembly as 2D hexagonal close-packed (hcp) arrays.

II-17

## **Unsymmetrical Phosphatidyl Choline Derivatives for Use as 2-D Surfactants in Monolayer Films**

**Zhongcheng Zhang,<sup>1</sup> Daniel K. Schwartz,<sup>2</sup> and T. Randall Lee<sup>1,\*</sup>**

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This presentation describes the synthesis and study of linactants (line-active molecules) for use as two-dimensional surfactants. Our first generation linactants are unsymmetrical phospholipids having chemically dissimilar tail groups. Specifically, intramolecular immiscibility is designed to arise from an incompatibility between dissimilar hydrophobic tails. When mixed with corresponding single-chain surfactants in a Langmuir-Blodgett architecture, linactants play a role in two-dimensional monolayers analogous to that which surfactants play in bulk three-dimensional systems. In particular, linactants can be used to stabilize lithographically-defined nanoscale structures that are the two-dimensional analogs of self-organized bulk materials that form due to amphiphilic self-assembly, such as micelles, emulsions, and lyotropic liquid crystalline phases.

## **Friday, February 9**

### **08:30–09:30 Session 5: Carbon Nanotubes**

*Professor Matteo Pasquali  
(Rice University), Chair*

08:30–08:50

## **Novel Nanocomposites Derived from Dispersed Multi-walled Carbon Nanotubes in Polymers: Micro-mechanisms of Deformation, Conduction Percolation, and Nanotube Crosslinking via Surface-Graft Polymerization**

**Arnold C.-M. Yang**

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A new class of nanocomposites that promises high toughness, excellent conductivity, and light weight was pursued by dispersing surface-grafted multiwalled carbon nanotubes in host polymers. The mechanical strength was found to increase dramatically when a small fraction of nanotubes were added in the glassy polymers, which clearly was resulted from alternation of micro-drawing mechanisms of the deformation zones. The nanotubes, too rigid to be drawn into large extension, piled up at zone boundaries, restricted widening of the deformation zones, and forced nucleation of new ones, resulting tremendous strength enhancement. The retardation of chain drawing, however, did not lead to transition of deformation mode from



crazing to yielding. It eventually prohibited large-scale plastic deformation, when nanotubes fraction increased, and brittleness prevailed finally. The capability of carbon nanotubes to be drawn into large extension emerged to be a key factor deciding whether full mechanical reinforcement could be realized. Homogeneous nanotubes dispersion promoted electric conductivity of the nanocomposites, which was found to follow percolation models. However, the micro-contact zones between percolated nanotubes were found to play a crucial role in imparting nanotube conductance to the composites. Only the nanotubes grafted with conductive polymer were able to construct nanocomposites with excellent electric conductivity as promised by percolated nanotubes. To exploit the intrinsic strength of carbon nanotubes and to create a covalently bonded nanotubes network for novel electric and optoelectronic properties, various synthesis methods were experimented to crosslink carbon nanotubes with long polymer chains. Gels of carbon nanotubes were ultimately synthesized that show interesting prospects.

08:50–09:10

## Portable Neutron Generator with ion source based on Carbon Nanotubes

Jiarui Liu and Wei-kan Chu

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Portable neutron generators are widely used in different areas such as explosives and weapon grade uranium detection, well logging and in-field activation analysis. Present portable neutron generators, like MP-320 (Thermo Electron), can provide neutron yield of  $10^6 - 10^8$  n/s.

Our new portable neutron generator is based on field ionization ion source with carbon nanotubes at room temperature. The yield of 14 MeV D-T neutrons is at  $10^{10}$  n/s level, which is higher than present portable neutron generators by 3 orders of magnitudes and comparable with movable neutron generators. In this neutron generator, the field ionization source is used to avoid the high power consumption in conventional plasma ion source. One HV power supply of about 100 kV is used for both ion source and acceleration. The main features of this kind of neutron generators are lightweight, lower power consumption, long lifetime, and easy maintenance. In neutron generators with solid Ti-T target, high beam power density will cause the T desorption and short target lifetime. The defocused ion beam or scanned ion beam can be used for long lifetime of the neutron generator. Our field ionization ion source provides non-focused Deuterium ion beam of mA in an area of  $\text{cm}^2$  with

the correspondent neutron yield of  $10^{10}$  n/s. Further optimization of the field emitters is in progress.

09:10–09:30

## Electronic Conduction in Single-Wall Carbon Nanotubes

Amir Farajian

*Rice University  
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09:30–09:45 Break

## 09:45–11:30 Session 6: Nanostructured Sensors

*Professor Huey Liang Hwang (National Tsing Hua University), Chair*

09:45–10:10

## Generating and manipulating spins in semiconductors

David D. Awschalom

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Spin-orbit coupling in semiconductors relates the spin of an electron to its momentum, and provides a pathway for electrically initializing and manipulating electron spins for applications in spintronics and spin-based quantum information processing. This coupling can be regulated with strain in bulk semiconductors and quantum confinement in semiconductor heterostructures. We provide an overview of optical studies exploring spin dynamics in conventional semiconductors, followed by recent experiments probing the all-electrical generation and manipulation of spins. Using magneto-optical spectroscopies with temporal and spatial resolution, new phenomena including current-induced spin polarization and the spin Hall effect have been observed in bulk semiconductors and heterostructures. These effects have recently been exploited to electrically generate on-chip spin currents that exceed the spin diffusion length and propagate macroscopic distances in the solid state. Surprisingly, both of these phenomena are observed over a broad range of temperatures and persist to room temperature in some materials despite no evidence for electrically-induced internal magnetic fields and notably weak spin-orbit coupling. Finally, we present experiments in diamond – a wide bandgap semiconductor – using angle-resolved magneto-

photoluminescence microscopy to image and manipulate single electron and nearby nitrogen spins at room temperature. These experiments enable the polarization and readout of single and coupled spins for information processing. The remarkable ability for all-electrical spin control at room temperature suggests that low power spin-based logic is technologically feasible in semiconductor devices.

10:10–10:30

## Thiophenol-modified CdS nanoparticles enhance the luminescence of benzoxyl dendron-substituted polyfluorene copolymers

Chia-Hung Chou<sup>1</sup>, Hsu-Shen Wang<sup>1</sup>, Kung-Hwa Wei<sup>1\*</sup>, and Jung Y. Huang<sup>2</sup>

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Highly luminescent dendron-substituted copolyfluorenes that incorporate surface-modified cadmium sulfide nanoparticles have been prepared. A small percentage of these nanoparticles can be incorporated into the dendritic structures upon tailoring the interfaces between the ligands on the nanoparticles and the dendritic structures in the copolyfluorene. Both the photoluminescence and electroluminescence efficiencies of the polymer nanocomposites are dramatically enhanced-sometimes more than doubled-relative to the values of the pure polymer.

10:30–10:50

## Shape-Controlled Synthesis of Metallic Copper Pyramids for Electrocatalytic Reduction of Nitrite Ions

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Free-standing pyramidal Cu nanoparticles have been synthesized in large quantities (over 90 %) on Au surface by

using electrodeposition process. It has been found that the concentration ratios of dodecylbenzenesulfonic acid sodium salt (DBSA) to Cu ion played an important role for the formation of Cu pyramidal islands. FESEM images reveal that the edge lengths of Cu pyramids range from 100 to 800 nm. Electron diffraction pattern shows that they crystallized in face-center-cubic (*fcc*). As an efficient electrocatalytic sensor, Cu nanoparticles were electrochemically grown on top of self-assembled 1-decanethiol (thio) layers on Au surface. The Cu NPs/thio/Au modified electrode shows high electrocatalytic activity for the reduction of NO<sub>2</sub><sup>-</sup> and exhibits a good reproducibility and stability. The catalytic peak current is found to show linear relationship with the nitrite concentration in the range of 0.001 – 0.3 mM with a correlation coefficient of 0.994. The detection limit approaches ~ 10<sup>-5</sup> mM and the response time is less than 2 seconds.

10:50–11:10

## Multifunction Nanoparticle-Nanotube/Nanotip Composites and Micro-devices for Energy and Sensing Applications

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Interactions between the electromagnetic wave, molecules and the noble-metal nanoparticles (NPs) having different shape, size and geometric arrangement result in many interesting physical and chemical properties, including surface enhanced Raman scattering (SERS), surface plasmon resonance and enhanced catalytic reaction. Nanoscale engineering and strategies that exemplify these novel properties will be presented in two cases: (1) dispersing metal NPs on the arrayed carbon nanotubes (CNTs) for electrochemical energy applications; (2) dispersing metal NPs on the arrayed Si nanotips for molecular sensing applications. For the first case, direct growth approaches of both NPs and CNTs were employed. Nitrogen incorporation in CNTs, whose structural behavior was understood in atomic level [*JACS* 2006], has played a key role in controlling the distribution and size of Pt/Ru NPs to enhance their catalytic activity and electron kinetics in the electrochemical environments. Such micro-device platform established in our lab has shown superior current collection efficiency and is amenable for energy applications [*J. Power Sources* 2006]. For the second case, well-aligned Si nanotip arrays with ultrahigh tip density were prepared by single-step electron cyclotron resonance plasma process at first [*US Patent* 2005]. These sub-wavelength nanostructures exhibit extraordinary broadband (from UV to FIR) antireflection properties, which

are only partly explainable by gradient index model, however. Moreover, when dispersed (*via* simple sputtering technique) with Ag NPs, they show excellent SERS properties. By optimizing the size of Ag NPs and their inter-particle distance, SERS of 8-order has been achieved, suggesting potential application of Ag NPs-dispersed nanotip arrays as molecular sensors.

11:10–11:30

## Flow Loop Experiments using Nanofluid Coolants

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Experiments were performed using a flow loop apparatus to explore the performance of nano-fluids in cooling applications for aircraft thermal management. The experiments were performed using exfoliated graphite nano-particle fibers suspended in Poly-Alpha-Olefin oil at mass concentrations of 0.6% and 0.3%. The experimental set-up consisted of a test section containing plain offset-fin cooler apparatus (gap fin or non-gap fin) which was connected to a flow loop consisting of a gear pump, a shell and tube heat exchanger (which was cooled or heated by constant temperature bath chiller/heater), and a reservoir. Experiments were conducted using nanofluid for two different fin strip layouts. Heat transfer data were obtained by parametrically varying the operating conditions (heat flux and flow rates). The heat transfer data for nanofluids were compared with heat transfer data for pure fluid under similar conditions. The change in surface morphology of the fins was investigated using Scanning Electron Micrography. The nanofluid properties were measured. It was observed that the viscosity is ~10 times higher for nanofluids and was found to increase with temperature. Specific heat of nanofluid was found to be 50% higher and was found to increase with temperature. The thermal diffusivity for nanofluids was found to increase with temperature and was measured to be 4 times higher. It was found that the convective heat transfer was enhanced by ~10% using nanofluids. Microscopy measurements show that the nanofluids deposit nano-particles on the surface which act as enhanced heat transfer surfaces (“*nano-fins*”).

Cleared as AFRL-WS 07-0132.

11:30–13:15 Buffet Lunch

## 13:15–14:45 Session 7: Mechanical Properties of Nanostructures

Professor Rui Huang (University of Texas), Chair

13:15–13:45

## Superplasticity and mechanics of carbon nanotubes

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Strength limits and mechanism of yield to deformation in carbon (C) and boron nitride (BN) nanotubes has been of great interest over the last decade. Advances in atomistic modeling have made possible quantitative mapping of these mechanical properties. Recent series of experimental observations of surprisingly plastic response to tension (e.g., up to threefold elongation!) can partially be explained by the early theory of the 5/7 dislocation glide. However important details like significant loss of mass through concurrent sublimation and also too high rates of plastic deformation at the temperatures in some cases much lower than sublimation, pose significant further problem for theory. We present complete kinetic description, based on calculation of energy and barriers for the elementary processes, detailed structural evolution, and phenomenological plasticity equations. Notably, it explains how the perfection of the lattice can be preserved, and how the radiation process serves as amplifier for the plastic yield rate.

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13:45–14:05

## The Development of Nano-Mechanics and Its Applications for Characterizing the Mechanical Property of Nano-Structures

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This presentation will introduce various computational algorithms for nano-mechanics including molecular dynamics and energy minimization. These computational approaches were used for nanoindentation technique to characterize the mechanical property of nanostructures. Applications including mechanical property characterization of nano-scale thin films, nanotubes and bio-materials will be discussed.

Nanoindentation has evolved to be a powerful means of characterizing mechanical properties through analysis of the load-depth curve obtained during nano-scale indentation. This presentation describes the nanoindentation using the depth-sensing technique for the characterization of the nano-structure. A molecular statics approach that is computationally efficient and can better reflect the physical reality during simulation will be introduced. With this approach, the mechanism of the elasto-plastic deformation can be examined more easily without the fluctuant motion of atoms. The simulation results show that the microscopic plastic deformation in the nano-scale thin film during indentation is caused by the instability of the crystalline structure. Homogeneous dislocation nucleation, glide and reactions are observed by virtue of slip vector analysis.

The validity of strain-gradient theory and applicability of the Oliver-Pharr method representing elastic-plastic continuum contact model are also examined. Moreover, the applications of nano mechanics and nanoindentation technique to the investigation of nanotubes, nanowires and bio-materials will be discussed.

14:05–14:25

## Investigation of Chromium Carbide/Alumina Nano-composite Prepared via MOCVD in Fluidized Bed

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Nanoscaled  $\text{Cr}_2\text{O}_3$  powder with an average particle size of 20~40 nm, coated on alumina particles, has been produced by means of chemical vapor deposition (CVD) in a fluidized chamber, using the pyrolysis of  $\text{Cr}(\text{CO})_6$  precursor. The precursor decomposed and formed the mixture of  $\text{CrC}_{1-x}$ ,  $\text{Cr}_2\text{O}_3$ , and free carbon on the surface of the  $\text{Al}_2\text{O}_3$  particles when paralyzed in fluidized bed. Amorphous and crystalline  $\text{Cr}_2\text{O}_3$  particles were obtained when the temperature of the pyrolysis were 300°C and 400 °C, respectively. The particles of decomposed  $\text{Cr}(\text{CO})_6$  treated at temperatures from 700 °C to 1000 °C in the graphite furnace in a vacuum were not carbonized until at 1150 °C. Amorphous  $\text{Cr}_2\text{O}_3$  powder were carbonized and transformed into  $\text{Cr}_3\text{C}_2$ , while the crystalline  $\text{Cr}_2\text{O}_3$  was transformed into a mixture of  $\text{Cr}_7\text{C}_3$  and  $\text{Cr}_3\text{C}_2$  under same thermal treatment. As  $\text{Cr}_2\text{O}_3$  react with  $\text{Al}_2\text{O}_3$  to form a solid solution and also it react with carbon to transform into chromium carbide, solid solution ( $\text{Cr}_2\text{O}_3$  /  $\text{Al}_2\text{O}_3$ ),  $\text{Cr}_3\text{C}_2$ , and  $\text{Cr}_7\text{C}_3$  were formed in this study. Combination of solid solution and nanosized 2<sup>nd</sup> phase reinforced were used for strengthening  $\text{Al}_2\text{O}_3$  base composites. From the observation in the microstructure of these high pressed specimens, the nanosized Cr-carbide particles disperse uniformly on the  $\text{Al}_2\text{O}_3$  grain boundaries and it can strengthen  $\text{Al}_2\text{O}_3$  matrix and suppress its grain growth. Comparing with the monolithic alumina, the mechanical properties of these nano-composites such as flexible strength and toughness significantly improved.

14:25–14:45

## The Tensile Properties of Single-wall Carbon Nanotubes

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Nanoscale tensile tests were performed on individual single-wall carbon nanotubes (SWCNTs) with a custom-made nanomanipulator inside the vacuum chamber of a scanning electron microscope (SEM). Freely-suspended individual SWCNTs were clamped to an atomic force microscope (AFM) cantilever probe with the electron beam induced deposition (EBID) method, and were loaded in tension until fracture. The AFM cantilever served as the force-sensing element. The applied tensile load was increased in discrete steps, and an SEM image was taken at each step. From image analysis the cantilever deflection and the nanotube elongation were obtained, and the tensile load and the strain were calculated. The diameter and chirality of each SWCNT were characterized with a Rayleigh scattering method prior to the test, and the tensile stress in the nanotube was calculated. A stress/strain curve was thus obtained, from which the fracture strength, failure strain, and elastic modulus of each SWCNT were obtained. In 9 samples the SWCNTs after loading to some value, slipped at the clamp on the AFM tip—a rather interesting result, but not allowing for study of fracture of these samples; the measured maximum tensile stress is only a lower bound of the true fracture strength. For the 13 SWCNTs tested that could be fractured failure always occurred at the EBID clamps, possibly due to stress concentration at the clamps or perhaps due to damage that might occur during EBID clamp formation; further study of these issues is indicated. The measured fracture strength values were 20 - 60 GPa.

**14:45-15:00 Break**

**15:00 All Posters Taken Down**

**15:00–16:20 Session 8: Nanostructures for Computing & Sensing**

*Professor Yeau-Ren Jeng (National Chung Cheng University), Chair*

**15:00–15:20**

## **Ferroelectric Micro- and Nanophotonic Structures and Devices**

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We report on the observation of single-mode stimulated bandedge emission from optically pumped prism-shaped gallium nitride (GaN) submicron-cavities. These cavities are fabricated by reaction-rate limited photo-chemical etching that preserves the non-polar  $\{10\bar{1}0\}$  or  $\{11\bar{2}0\}$  facets. The cavities are characterized to have an average quality factor of  $10^3$  and facet reflectivity exceeding 99%, allowing field-amplification due to repeated reflections in the transverse plane and field-polarization along the  $c$  axis. The demonstrated Q of this cavity is comparable to the state-of-the-art GaN nano-ring structure that has required sophisticated manipulation to fabricate.

PPLT is a ferroelectric material that has promise of efficient wavelength conversion to the blue and uv regions. We have fabricated 2D quasi-phase-matched structures using PPLT and demonstrated efficient (>30%) SHG to the red, green, and blue wavelengths with these structures. We have also demonstrated a near-room temperature visible parametric oscillator capable of emitting 1W average power. This leads to the design and construction of a monolithic white light source that could have unity pump to white light conversion efficiency.

**15:20–15:40**

## **Self-assembly of micro-retroreflectors**

**Steven M. Kemper<sup>1</sup>, Kaajal D. Shah<sup>1</sup>, Tim Sherlock<sup>2</sup>, Paul Ruchhoeft<sup>2,†</sup>, Robert L. Atmar<sup>3</sup>, and Richard C. Willson<sup>1,4,‡</sup>**

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Modern bioanalytical technologies, ranging from DNA probe array monitoring of mRNA expression to immunoassays for clinical diagnosis and biodefense, rely upon labels attached to biomolecules to make them easily detectable. Currently, the most common labels are fluorescent dyes, which emit a known wavelength of light when excited by shorter-wavelength radiation. Although extremely useful and well developed, such systems can suffer from low signal strength, low signal to noise ratios, low quantum efficiency, and photobleaching.

We are developing a new and potentially superior label system based upon corner-cube micro-retroreflectors. Such retroreflectors consist of transparent cubes with three mirrored surfaces and return incident radiation directly back its source,

making them extremely detectable. In fact, a set of corner-cube retroreflectors on the lunar surface is routinely detected and ranged as part of ongoing experiments on lunar orbital dynamics. Miniaturizing such a system would allow for the fabrication of labels with potentially superior performance in immunoassay, cell sorting, and microarray applications.

Currently, we fabricate micron-sized corner cubes on glass silicon wafers where one of the three reflective surfaces is decorated with antibodies that capture the target molecule. Gold nanoparticles, also decorated with anti-target antibodies, assemble on the surface in the presence of the target molecule and substantially reduce the surface reflectivity at specific wavelengths. Because the surface area is very low (tens of square microns), the device sensitivity is potentially very high. We are currently addressing the rapid detection of Norwalk virus in collaboration with researchers from the Baylor College of Medicine.

15:40–16:00

## Nano-Fabrication assisted by x-rays

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Assisted by the high coherence of synchrotron X-rays, phase contrast due to the difference in the refractive index is added to the absorption as another, yet much improved, contrast mechanism. Together with the improvement in the detecting system, we can now looking deep inside into matters with unprecedented precision and speed. Sub- $\mu\text{m}$  or better resolution radiograph can now be obtained with ease and in many cases fast phenomenon can be observed with time resolution better than tens of microsecond. Ongoing developments in the instrumentation and reconstruction algorithms have generated higher excitement with the recent demonstration of 30nm scale resolution in 3D.

The intense x-rays are also used to fabricate nanostructures, mostly by x-ray lithography and LIGA techniques. The similar x-ray-induced chemical reactions can also be used to synthesize nanoparticles of metals, oxides and polymers with great efficiency and control. These previously unknown capabilities of x-rays now open the door to a number of new therapeutical methods which relies on x-ray targeted drug release, enhanced x-ray radiotherapy and microbeam therapy. These new therapeutical strategy might be relevant human health in the near future. Together with the much better know capability of x-ray in characterization—x-ray diffractions, x-ray absorption spectroscopy, a short review of x-ray technology will address specifically its application to various

domains in science, the relevance to the medicine, nano-science and -technology.

16:00–16:20

## Nerve Agent and Chemical Sensing Using Nanostructured Crosslinked Dendrimeric Precursors

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This work describes the use of nanostructured conjugated crosslinked polymer materials based on PAMAM dendrimer precursors that have very high selectivity and sensitivity for toxic nerve agents. These nerve agents based on organo-phosphate derivatives such as sarin and soman are highly toxic and yet can be practically indistinguishable from organophosphate fertilizer derivatives in terms of chemical identification. By using electrochemically crosslinked dendrimer precursors with carbazole peripheral groups, highly sensitive and selective sensing was achieved using a surface plasmon resonance technique (SPR) on nerve agent analogs. The sensitivity was found to be from nanomolar to picomolar values. The nanostructure of the ultrathin films was achieved by a carefully controlled dendrimer design as well as the incorporation of  $\text{Cu}^{++}$  ions together with a self-assembled monolayer (SAM) modified substrate. The possibilities for using nanopatterned substrates will be demonstrated. The importance of material nanostructure and composition parameters is emphasized.

16:20

## Closing Remarks

*Dr. Harold Weinstock (AFRL/AFOSR)  
and Prof. M. K. Wu (Academia Sinica)*

18:00

## Optional Evening Event

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