Electronics
Room 312 - Session EL+NS-TuM
Molecular Electronics

Moderator: Y. Liang, Pacific Northwest National Laboratory

8:20am **EL+NS-TuM1 Molecules, Hierarchical Assembly and Architecture of Moletronic Computers***, **W.L. Warren**,* Defense Advanced Research Projects Agency **INVITED**

While the rapid miniaturization of electronics has driven much of the development of computation and information systems, it is anticipated that future computational demands for performing calculations orders of magnitude faster with less power. To create discovery beyond silicon, the DARPA Moletronics program is proposing that both computational functionality and input/output architecture can be designed in molecular systems. These systems will high device density (scaleable to 10@super 12@ device/cm@super 2@) and be amenable to greatly simplified manufacturing fabrication using hierarchical-assembly. It is anticipated that architecture, a top-down approach will play an immense role in steering discovery. Moletronics is focussed on developing technologies based on the self-assembly of molecular components to act as devices, switches, and interconnects. The program does not clone contemporary electronic devices with molecular scale components, but rather create functionality that exploits what molecules are good at (self-assembly, thermodynamic equilibrium, and charge storage media.) The trick for molecular computers will be to cope with defects and to realize hierarchical processes to manufacture the hardware. Hierarchical assembly is envisaged as a set of processes that will first assemble individual devices, then create functional blocks (circuits) from those devices and finally assemble systems from the blocks. It is a bottom-up manufacturing process whereas current microelectronics fabrication is based on top-down manufacturing using lithography. The talk will discuss three over-riding themes of the Moletronics program: (1) molecular devices, (2) hierarchical assembly, and (3) architecture including defect tolerance and algorithm development to find the defects. @FootnoteText@ @footnote 1@ The contributions of the contractors of the DARPA Moletronics program and fellow program managers, Bruce Gnade, Christie Marrian, and John Pazik are gratefully acknowledged.

9:00am **EL+NS-TuM3 Molecular Wires, Switches and Memories***, **J. Chen**,* Yale University **INVITED**

Molecular electronics has recently attracted much attention because of its potential application in future computational systems. Molecular wires and related strategically engineered structures (e. g., molecular switches and memories) offer an increased versatility in device design with reduced elements. Nanoscale molecular devices utilizing active self-assembled monolayer (SAM) as the active component will be reported. We will present results on: (1). measurements of through-bond conductance of symmetric metal/conjugated SAM/metal junctions where non-Ohmic thermionic emission was observed to be the dominant process, with isocyanide-Pd contacts showing the lowest thermionic barrier of 0.22 eV; (2). first realization of robust and large reversible switching behavior in an electronic device that utilizes molecules containing a nitroamine redox center (2'-amino-4,4'-di(ethynylphenyl)--5'-nitro-1-benzenethiolate) exhibiting negative differential resistance (NDR) and an on-off peak-to-valley ratio (PVR) exceeding 1000:1; while molecules containing a nitro-only redox center (4,4'-di(ethynylphenyl)-2'-nitro-1-benzenethiolate) exhibiting room temperature NDR; (3) demonstration of a two-terminal electronically programmable and erasable molecular memory cell with bit retention time greater than 10 minutes.

9:40am **EL+NS-TuM5 Dissimilar Metal Electrodes with Nanometer Interelectrode Distance: Fabrication and Application to Characterizing Self-Assembled Molecular Electronic Devices***, **M.A. Guillorn**, I. Lee,* University of Tennessee*; D.W. Carr, R. Tiberio,* Cornell Nanofabrication Facility*; E. Greenbaum, J. Lee,* Oak Ridge National Laboratory*; M.L. Simpson,* Oak Ridge National Laboratory and The University of Tennessee

In order to advance the state of molecular-scale electronics research, electrode structures capable of realizing metal/molecular monolayer/metal heterojunctions have been fabricated using a variety of novel techniques that allow direct electrical contact with single molecules and small groups of molecules. By using Au as the electrode material, thiol-based self-assembly techniques have been successfully applied to deposit organic-synthetic molecules between these electrodes, thereby permitting their electrical characterization. This is possible due to the symmetry of these molecules. Unfortunately these techniques do not lend themselves to measuring the electrical properties of asymmetric molecules. An example of this type of molecule is the Photosystem I (PSI) reaction center which is of demonstrated interest to molecular-scale electronics research. Self-assembly techniques have been developed to preferentially orient the PSI with respect to a Au substrate, however, the polar nature of this molecule inhibits the use of this technique for the formation of Au/PSI/Au heterostructures. In this paper we will discuss a flexible and reproducible process for fabricating dissimilar metal electrodes with nanometer interelectrode distance (DiMEND) using high-resolution electron beam lithography and liftoff pattern transfer. This process is capable of realizing electrode pairs with a minimum interelectrode distance of less than 6 nm. This technique provides a reproducible method for creating lateral structures well suited for the electrical characterization of asymmetric molecules for molecular-scale electronics applications. Applications of this technology to characterizing self-assembled molecular electronic devices will be presented.

10:00am **EL+NS-TuM6 Characterization of Gold/Pentacene and Pentacene/Gold Interfaces***, Q.T. Le, S. Zorba, E.F. Forsythe, L. Yan, **N.J. Watkins**, Y. Gao,* University of Rochester*; S.F. Nelson,* Colby College*; C.S. Kuo, T.N. Jackson,* The Pennsylvania State University

Among the conjugated oligomers used as active materials in the fabrication of organic thin-film transistors (OTFT), pentacene is one of the most promising materials due to its high field-effect mobility. The performance of pentacene based OTFTs is now comparable to that obtained from hydrogenated amorphous silicon TFTs. The interface formed between the organic semiconductor and the conducting layer strongly influences the current-voltage characteristics of OTFTs. We report the interface formation between gold (Au) and pentacene using x-ray and ultraviolet photoelectron spectroscopy (XPS and UPS). The morphology of the pentacene film deposited on the substrate was measured using atomic force microscopy, showing a pentacene layer with small grain size. XPS results indicate that Au does not chemically react with pentacene if Au is deposited onto pentacene or if pentacene is deposited onto Au. For Au deposited on pentacene the UPS results show that there is an initial binding energy shift of both the highest occupied molecular orbital of pentacene and the vacuum level attributed to the formation of a common fermi level for the Au and pentacene as the Au is deposited. The initial increase is then followed by a decrease in binding energy shifts that is attributed to a reduction of the polarization energy caused by the formation of a Au overlayer on the surface of the pentacene. For pentacene deposited onto Au the UPS results show that there is only a shift of the vacuum level to lower binding energy.shift of the vacuum level to lower binding energy.

10:20am **EL+NS-TuM7 Current-Induced Organic Molecule-Silicon Bond Breaking: Consequences for Molecular Devices***, **S.N. Patitsas**, G.P. Lopinski, O. Hul'ko, D.J. Moffatt,* National Research Council of Canada*; R.A. Wolkow,* National Research Council of Canada, Canada

The current carrying capacity of individual organic molecules covalently bound to silicon has been studied. Adsorbates comprised exclusively of saturated C-C bonds were found to be entirely stable whereas adsorbates containing pi-bonds could be controllably dislodged under modest conditions. The pi-bonds act as a chromophore, taking energy from a scattered electron, energy that can be selectively channeled into Si-C bond breaking. The class of adsorbates that are dislodged is closely related to unsaturated molecules widely investigated for enhanced molecular wire character. It is predicted that molecular devices containing such molecules will fail when operated. Measures to avoid current-induced bond breaking are described. New processes based upon the controlled bond breaking phenomenon are suggested.

10:40am **EL+NS-TuM8 Molecular Arrays and Individual Dopants Studied by Ultrahigh Vacuum Scanning Tunneling Microscopy***, **L. Liu**, J. Yu, N. Viernes, M.C. Hersam, N.P. Guisinger, J.W. Lyding,* University of Illinois

One aspect of molecular electronics is the fabrication of atomically precise molecular arrays on silicon substrates. Feedback controlled lithography (FCL) is used in conjunction with UHV STM to create atomically precise templates for molecular adsorption. Cobalt phthalocyanine (CoPc) molecules have been sublimed onto these templates and subsequently imaged in the STM. The difference between filled state and empty state images is explained. Current imaging tunneling spectroscopy (CITS) of CoPc is also performed and discussed. CoPc Molecular symmetry as well as the feature associated with the central Co atom are studied in all STM images. CITS has also been used to identify and study individual dopants on or near

Si(100)2X1:H surfaces. For high quality UHV H-passivated Si(100) the Fermi level is unpinned at the surface, thus enabling the observation of subtle features including subsurface dopants. For example, boron atoms appear as slight hillocks in filled state images and as centro-symmetric depressions in empty states. Full CITS data sets and their analysis and interpretation will be presented. The same techniques will be used to present results for isolated Si dangling bonds created by FCL.

11:00am **EL+NS-TuM9 Direct Measurements of Electrical Transport through DNA Molecules***, **D. Porath**,* Tel Aviv University, Israel & Delft Univ. of Tech., The Netherlands, Israel*; A. Bezryadin,* Harvard University*; S. de Vries, C. Dekker,* Delft University of Technology, The Netherlands **INVITED**

Is DNA a conductor for electrical charges? This question has been heavily debated over the past few years, spurred by optical experiments that measured fluorescence quenching for DNA molecules and recent electrical measurements. Here we present measurements of electrical transport through short and well-defined DNA molecules that show large-gap semiconducting behavior. A 10.4 nm long, double-stranded poly(G)-poly(C) DNA molecule is connected to two metal nanoelectrodes that are separated by 8 nm. Nonlinear current-voltage curves with a voltage gap at low bias are observed at ambient conditions as well as in vacuum and at cryogenic temperatures. The voltage dependence of the differential conductance exhibits a peak structure, suggesting that transport of charge carriers is mediated by the molecular energy bands of DNA. Recent STM measurement on similar DNA molecules will be shown as well.

11:40am **EL+NS-TuM11 Whole-Cell Bio-computing in a Microelectronic Format***, **M.L. Simpson**,* Oak Ridge National Laboratory and The University of Tennessee*; G.S. Sayler, J. Fleming, B. Applegate, S. Ripp, D. Nivens,* University of Tennessee Center for Environmental Biotechnology

Even simple cells perform tremendously complex information processing operations involving memory (genes), sensing and feedback (promoters, regulatory proteins), and in some cases, interconnectivity (quorum sensing). For example, Escherichia coli, with a 4.6 million base-pair chromosome, has the equivalent of a 9.2-megabit memory to code for as many as 4,300 different polypeptides under the inducible control of perhaps several hundred different promoters. Yet, all of this functionality is contained in an area of approximately 1 square micron. Conversely, current predictions of the future of silicon integrated circuits indicate that 1 square micron of silicon will contain only a 245 bit memory or 1.66 simple logic gates by 2014. Obviously, silicon technology will not approach bacterial-scale integration within the foreseeable future. Furthermore, microorganisms have some qualities that are quite desirable for information processing devices and systems. Bacterial cells are relatively rugged "devices" that subsist in even extreme environments. Also, they are fairly easy to manipulate genetically, and have a diverse set of gene regulation systems. Furthermore, cells easily can be incorporated into a 3-dimensional structure instead of the planar structure of integrated circuits. And finally, cells self-assemble and self-replicate, and therefore are easy to manufacture. We will present our work to incorporate the information processing capabilities of living cells into a microelectronic format. This will include our work on the bioluminescent bioreporter integrated circuit (BBIC) for sensing applications, as well as our recent work to engineer more complex information processing and communication functions into whole cells deployed on integrated circuits.

Author Index

Bold page numbers indicate presenter