



# Friday Morning, November 17, 2006

10:20am **EM-FrM8 Fabrication of Semiconductor-Molecule-Semiconductor (SMS) Devices**, *A. Mahapatra, M. Martinez, P. Carpenter, A.D. Scott*, Purdue University; *A. Yulius*, Yale University; *J. Woodall, D.B. Janes*, Purdue University

Molecular electronic devices have typically been fabricated using metal-molecule-metal (MMM) configurations. Recently, several studies involving semiconductor-molecule-metal (SMM) junctions have been reported, motivated by the prospects of realizing covalent bonds to one contact and exploiting the semiconductor states in device properties. The MMM and SMM junctions are the commonly used device structures for studying the electrical behavior of single/few molecules. While the SMM structures address some of the problems with reliability of MMM structures, there is still the possibility of metal penetration through the molecular layer during deposition or device operation. This study illustrates a technique to fabricate large area molecular devices in a semiconductor-molecule-semiconductor (SMS) configuration by depositing a pre-formed semiconductor island (InAs) onto a molecular self-assembled monolayer (SAM) which has been formed on another semiconductor substrate (GaAs). Micron-scale InAs islands with Au top contact layers are formed on a sacrificial substrate and transferred onto the SAM-coated GaAs substrate. Identical topography of the grains on the surface of the settled islands and freshly prepared Au surfaces, confirm that the InAs side of the island is in contact with the SAM-coated GaAs surface. In order to verify that thiol-based bonds are possible on InAs (for the top contact), we have also developed SAMs of short thiol molecules on InAs surfaces. The resulting SAMs were characterized through X-ray photoemission spectroscopy. Electrical conduction has been measured for p@super +@GaAs/xylyl-dithiol/InAs structures of 100-400  $\mu\text{m}^2$  contact areas. This study demonstrates that molecular devices can be realized using exclusively semiconductor contacts.

10:40am **EM-FrM9 Molecular Tunnel Junctions Incorporating Nickel-Octanedithiol Multilayer Thin Film**, *L.H. Yu, J.G. Kushmerick*, National Institute of Standards and Technology

We present measurement of tunneling junctions made using self-assembled nickel-octanedithiol multilayer thin film. Multilayer structures on evaporated gold and nickel surfaces were studied by ellipsometry, Fourier Transform Infrared (FTIR) spectroscopy, and X-ray photoelectron spectroscopy (XPS). Superconducting quantum interference device (SQUID) measurements were performed on the nickel-dithiol multilayer thin films and bulk materials to characterize their magnetic properties. We will discuss the effect of applied magnetic field on the electronic transport of these ferromagnetic atoms containing tunneling junctions.

11:00am **EM-FrM10 Electrical Transport Measurements on Conjugated Molecules using Nanogap Electrodes on Cleaved AlGaAs Planes**, *M. Tornow, S.M. Luber, S. Lingitz, A.G. Hansen, F. Zhang*, Walter Schottky Institute, TU Munich, Germany; *F. Scheliga, E. Thorn-Csányi*, University of Hamburg, Germany; *M. Bichler*, Walter Schottky Institute, TU Munich, Germany

One of the major challenges in the realization of molecular electronic hybrid systems that comprise molecules as functional units is the reproducible fabrication of the inorganic contact electrodes. We have developed a novel technique to prepare such nanogap electrodes in a very precise manner, based on cleaved GaAs/AlGaAs semiconductor heterostructures grown by Molecular Beam Epitaxy (MBE).@footnote 1@ These electrodes of predetermined distance are macroscopically flat, coplanar and exceedingly clean. We report on electronic transport measurements on @pi@-conjugated, dithiolated Oligo-(phenylvinylene) (OPV) derivatives of length 8.5 nm bridging a ~7 nm nanogap device. Starting from a high impedance behaviour before molecule deposition the OPV functionalized hybrid system develops a pronounced non-linear I-V characteristic measured at T=4.2 K. We compare our observations to model calculations on a simplified structure involving extended Hueckel theory and non-equilibrium Greens Function methods, and find qualitatively good agreement. @FootnoteText@ @footnote 1@ S.M. Luber et al., Nanotechnology 16, 1182 (2005).

11:20am **EM-FrM11 Dynamics of Molecular Quantum-Dot Cellular Automata Devices and Circuits**, *Y. Lu, M. Liu, C. Lent*, University of Notre Dame

Quantum-dot cellular automata (QCA) provides a non-transistor alternative for the design of molecular electronics. Binary information is encoded in the charge configuration of molecular cells. Information is transported from cell to cell through the Coulomb interaction. Clocked control of molecular QCA can be accomplished by employing an applied clocking field

which varies regularly in both space and time. This enables binary information to be transported across molecular arrays without electrons moving between molecules. Power gain restores signal energy lost to unavoidable dissipative processes. Here we study dynamic properties of molecular QCA devices including energy dissipation, operating frequency, and defect tolerance. We use detailed quantum chemistry results for molecules to construct simpler effective Hamiltonians for each QCA molecular cell. We then solve the equation of motion of the whole molecular device using a coherence vector formalism which includes both quantum effects and dissipative coupling to the environment. This enables us to characterize non-equilibrium and finite-temperature effects on switching behavior. We explore the structure-function relation in molecular QCA at two levels: that of the individual molecules and that of the circuit layout. The specific character of the inter-dot intra-molecular linker plays a crucial role in the dynamics of molecular switching, particularly near the maximum possible switching speeds. At the level of the circuit as a whole, a key challenge for all molecular electronics is handling defects due to the fundamental thermodynamic inability to control exactly the position and orientation of each single-molecule device. The QCA approach has the advantage of being inherently robust against disorder and can be made even more so by simply using wider wires to build in redundancy.

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