Merged CMOS/Molecular Integrated Circuit Fabrication, Analysis, and Design

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Project overview: This project looks at nanoelectronics from a comprehensive viewpoint by considering how nano-devices and nano-circuits can be assembled, modeled and designed with the requirements of large-scale integration and manufacturability in mind[1]. Current microelectronics technology is dominated by silicon CMOS technology. As this technology is scaled to smaller dimensions and higher densities, eventually fundamental physical limits of MOS transistors will be reached. It is the hope of molecular electronics to replace the functionality of conventional circuits with new devices based single (or a small number) molecules. As with any new microelectronics technology, it is likely that molecular devices will be introduced in a somewhat gradual way. Molecular devices will be used for critical functions along with conventional CMOS for other functions. As the scale of integration increases, more and more of the functionality will shift to the molecular devices. The motivation for our program is to develop the underlying science and technology to enable integration of functional molecular devices with conventional electronics. It is then critical to understand materials compatibility and device performance issues at the outset. Our program includes efforts on molecular synthesis, basic device functionality, compatible materials and fabrication methods, device modeling, and higher level abstractions leading to functional circuit architectures. Our program is aimed at addressing these issues with a multi-disciplinary team spanning chemistry, chemical engineering, electrical engineering, and computer engineering.

Project Goals: One of the main goals of the project is to develop fabrication methods that allow for integration of molecular devices with conventional CMOS circuits. We envision this to be a back-end process where modern integrated circuits use a variety of metals (Al, Cu, Ta, W, Ti, etc.) and insulators (SiO_2, SiN, etc.) in multilevel metalization schemes that result in a complex 2.5 dimensional arrangement of contacts and wires. Near the end of the process sequence, the insulating layers would be etched away leaving pockets that by their shape, size and Cu endpoints, provide an ideal "home" for the target molecule. The completed template could then be rinsed in a solution containing these molecules, adding them to the structure. Since the volatile organics would not be subject to high temperature processing, this could provide a viable means of adding molecular electronic devices to underling microelectronic circuits.

Second, we have developed device models of molecular devices. These models are essential if one is to anticipate novel computing architectures where molecular devices may function far differently from modern transistors, and where optimized circuit design my entail radically different patterns of device interconnection. Ultimately, we hope to close the loop on the entire process and feed back our circuit level results to the efforts in molecular synthesis and design as well as fabrication.

Finally, a significant part of our effort is dedicated to education and outreach. The subject of nano-electronics is highly interdisciplinary and does not fall within the normal pedagogical bounds of engineering and scientific disciplines. We are developing a 3-D animation based website emphasizing the fundamentals of nano-device operation and integration.

Recent Results: A test structure for electrical characterization of metal-molecule-metal junctions was built using simplified processing tools and procedures. The test device consisted of nanometer scale well with a gold bottom, a self-assembled molecular monolayer on the bottom of the well, and capped with titanium/gold. The test device was similar to a device built by a group in Yale[2] but had simplifications in the area of processing tools and conditions. The device tested alkanethiol molecules that were found to tunnel electrons in metal-molecule-metal junctions. The parameters for tunneling, such as potential barrier height (ϕ_b) and barrier shape (β) were determined[3]. The values of these parameters are comparable to those found in the literature. An exponential dependence of tunneling current to the chain length was also found. The exponential decay factor calculated by experimenting with different chain length molecules agreed well with the literature values.

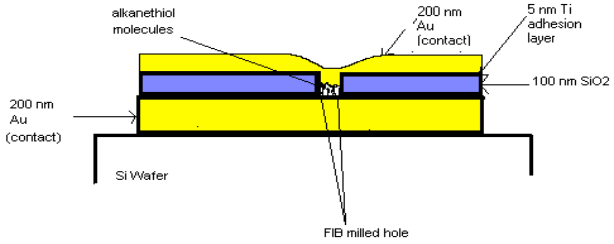

Figure 2 side view of our device..

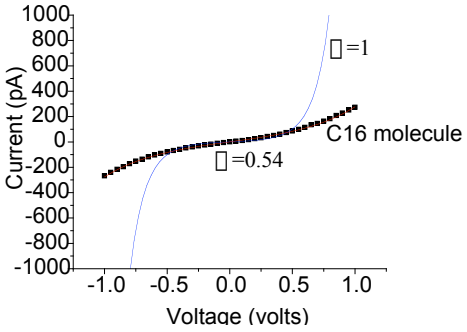

Figure 1 I-V plot shows c16 experimental data for c16 molecule. Blue line is the plot with a=1 and the red line is the theoretical fit for C16 with β=.54 confirming a nonrectangular fit. barrier height (ϕ_b)

Molecule	ϕ_b (V)	β
C16	2.1±0.1	.56±.02
C14	2.1±0.1	.56±.02
C12	2.1±0.1	.55±.05
C10	2.0±0.1	.75±.02
C8	2.1±0.1	.77±.05

Table 1. β values for different chain length molecules

Our simplified test structure will enable us to determine I-V characteristics and other fundamental measurements for a wide variety of molecular species. This device serves as a test bed for molecules designed and synthesized in our project. An example of such a molecule is shown in Fig. 4. This molecule consists of a tri-phenyl structure with specific attachment (R) groups on the center ring. Knowledge of basic transport and conduction mechanisms is critical for the advancement of molecular electronic devices.

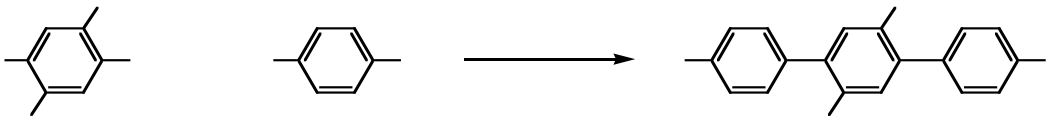

Figure 4 Example of a molecular synthesis for a tri-phenyl molecule with attachment groups.

We have developed a universal device model for molecular devices[5]. This model takes, as input, the electrical behavior (current vs. voltage) of a molecular structure and constructs a device model based on combinations of fundamental device behaviors. Figure 5 illustrates the case of a

negative differential resistance molecule[3]. The experimental data is used to extract device model parameters that can later be used in circuit models.

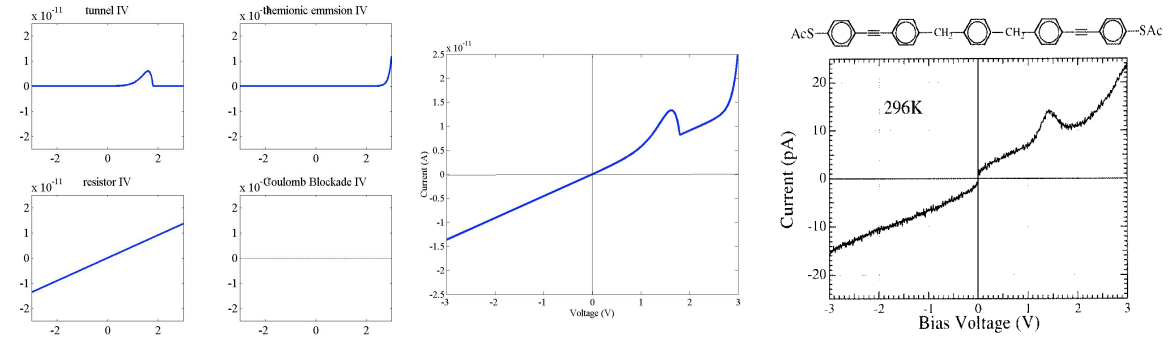

Figure 5 Universal Device Model parameter extraction example. The experimental data (far right) is fitted to a model that includes components of tunneling, thermionic emission, resistance and possible Coloumb blockade. The resulting model (center) can be used to extract parameters for circuit designs. The UDM is available for public download at
http://www.ece.virginia.edu/hplp/nano.html

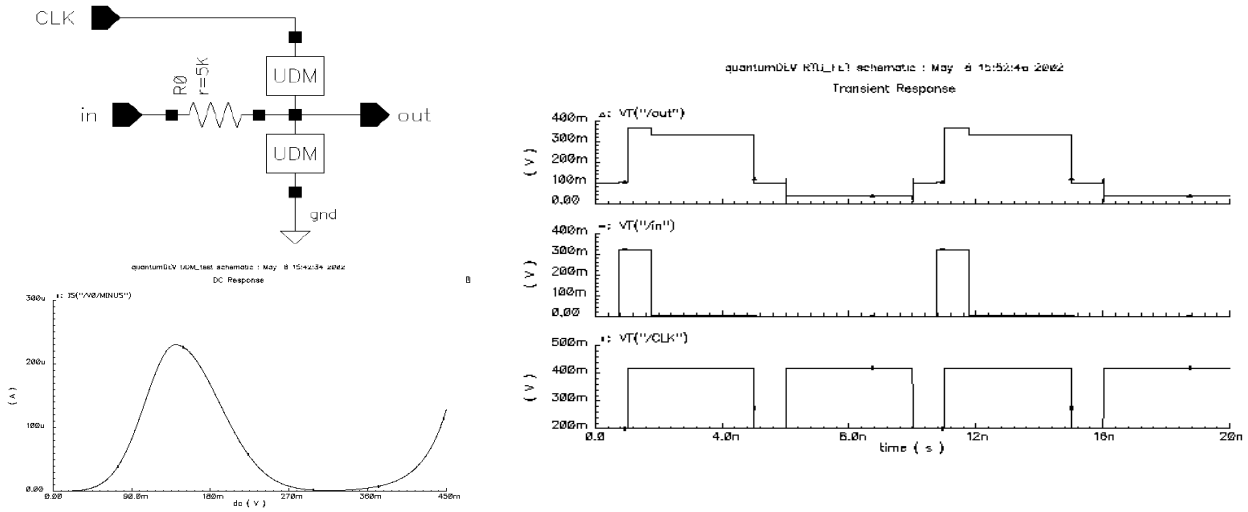

Figure 6 Latches with stacked negative differential resistance devices such as resonant tunneling diodes(RTDs) or the molecular functional equivalent can provide sequential logic as well as gain in molecular nanoelectronics
UDM model implemented in Verilog-A and simulated with the Spectre circuit simulator from Cadence

Figure 6 illustrates an example of a logic circuit (latch) implemented with an architecture using stacked negative differential resistance devices (such as the molecular structure in Fig. 5). The universal device model was used to extract parameters as input to a circuit model that demonstrated the functionality of the circuit.

References:

1. For further information on this project send e-mail to lrharriott@virginia.edu
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