Center for Electron Transport in Molecular Nanostructures

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The Center for Electron Transport in Molecular Nanostructures has been established at Columbia University with the primary purpose of developing the fundamental basis for understanding of the flow of charge through individual molecules and through molecular nanostructures in contact with metals held at defined potential differences [1]. The program is built upon Columbia University's strong expertise in both chemical synthesis and in fundamental charge transport phenomena, as well as upon a close collaboration with IBM and Lucent Technologies, leading industrial research programs at in electronic processing of information. The research program of the proposed Center may be best understood by the questions that we are addressing. These include basic, but largely unanswered, questions about electronic transport in molecular nanostructures including:

- What are the fundamental principles that determine the response of a molecular system to application of electric potentials through contact with electrode structures?
- How can we electronically contact molecular systems?
- What is the nature of the contact to individual nanotubes, molecules?
- How do we design insulators for molecular circuitry?
- What are possible mechanisms for modulation of the conductance of a molecule?
- How can we build three-junction molecules (or "molecular tripods") containing the operational functions of a transistor?

These and similar issues comprise questions underlying nanoscale molecular electronics, questions that must be addressed to make sustained progress at the frontier of nanotechnology. They are also questions of great inherent scientific interest and importance, ones that can be expected to impact other disciplines as well.

The Columbia Nanocenter's research program is structured into three primary parts. Two components focus on the fundamental aspects of electron transport in molecular nanostructures. These research directions provide fundamental insights into many remarkable scientific and technological advances in (1) carbon nanotube transport and (2) transport in thin film organic semiconductors and devices. The third component of the research program is directed more explicitly to single-molecule transport. We are fabricating single-molecule structures through a fusion of advanced semiconductor technology and tailored molecular synthesis. This research elucidates the control of charge transport through single molecules in terms of the chemical structure, but it also examines underlying mechanistic questions. Our research program places strong emphasis on the modulation of charge transport through molecules, with the goal of advancing the understanding and development of a three-terminal molecular transistor.

Charge Transport in Carbon Nanotube Structures. Members of our research team have demonstrated carbon nanotube (CNT) based electronic devices with excellent characteristics [2].

However much of the basic science underlying the operation of these devices remains to be discovered. We are interested in understanding such questions as: What is relationship between nanotube chemical structure and device properties? What is influence of chemical and physical defects in nanotube? How does chemical modification or the environment influence conduction properties? What is role of nanotube-metal junction? We have begun by building complete operating devices within the NSEC facilities. Figure 1 shows an electron micrograph of a single-wall CNT device prepared by synthesizing nanotube structures across lithographically-defined porous silica on a Si wafer with an SiO_2 insulator followed by deposition of electrodes through shadow evaporation. These devices allow us to measure and to understand the responses of these devices to various chemical and environmental conditions. Using these concepts for example we have found that the operation of these devices can be very strongly influenced by interaction with oxygen (see Figure 2) and through these studies we have begun to understand the nature of the nanotube/metal interface and its influence on conduction within the device.

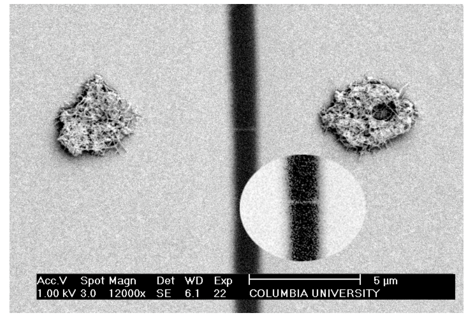

Figure 1. Electron micrograph of a carbon nanotube field effect transistor fabricated at Columbia University. (Takao Someya).

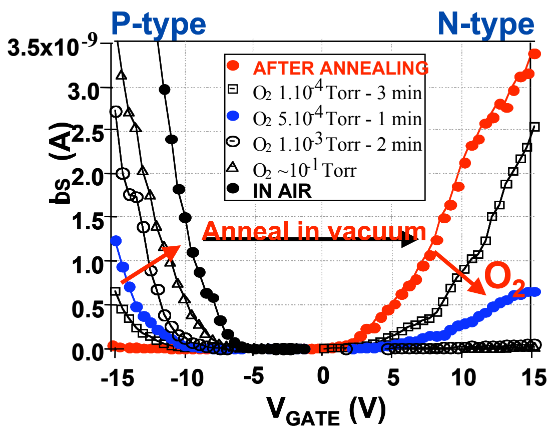

Figure 2. Conductance properties of carbon nanotube FET device subjected to different conditions. (Phaedon Avouris, Louis Brus, Xiaodong Cui)

Charge Transport in Molecular Nanostructures. Although organic semiconductors such as pentacene are known to be useful in thin film transistors and other thin film electronic devices, our understanding of the basic phenomena is very limited. Questions that concern the Nanocenter include: What is nature of conduction in organic nanocrystals? What is role of grain boundaries and crystal defects in semiconductor properties? What molecular properties, structures, and characteristics determine conduction properties? We have chosen to begin our studies on a very basic system: crystalline pentacene. We are growing single-domain pentacene nanostructures through physical vapor deposition (Figure 3). Thicknesses range from a single molecular layer to many layers. We are examining the charges that appear on these nanostructures and the charge dynamics. Our intent is then to examine photoconduction and field effect conduction changes in these single domain nanostructures.

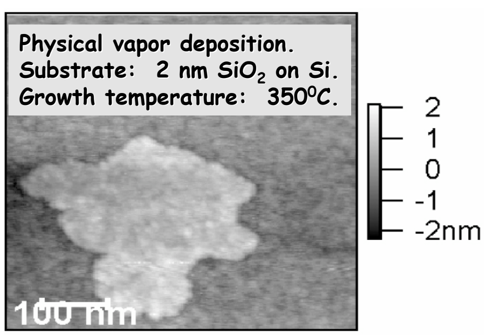

Figure 3. AFM topographical image of single domain pentacene nanocrystal of one molecular layer thickness. (Louis Brus, Cherie Kagan, Liwei Chen)

We are also exploring new molecular concepts for self-assembly of organic materials that may be useful for creation of new thin film and molecular devices. An example of this is a novel compound with strong hydrogen bonding designed to build up molecular stacks indicated in Figure 4. This compound for example spontaneously forms fibers on graphite surfaces including single molecule fibers and 3-molecule ropes. We are exploring the molecular structures in these

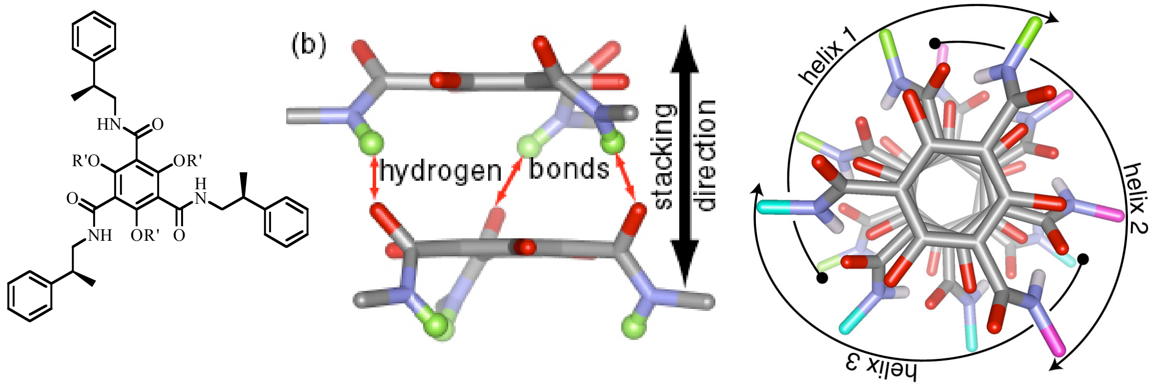

Figure 4. Chemical structure and anticipated molecular packing for typical molecular fiber compounds. (Colin Nuckolls)

systems. We are also investigating electron conductance in these systems as well as other applications in molecular devices. Members of the research team draw heavily on modern scanning probe techniques to study molecular structures on the molecular scale.

<u>*Charge Transport in Single Molecules*</u>. Our activity in molecular electronics is based on the following elements: build theoretical understanding, synthesize new molecules, fabricate suitable "sockets" for individual molecules, develop techniques for binding molecules to sockets, explore conduction properties, ultimately seeking 3-terminal architectures. Exemplary of the molecular systems under consideration is the structure shown in Figure 5 that combines chemical groups reactive with metals, a rigid highly conjugated backbone, and side-arms that provide for processing and ordering. We are actively engaged in developing theoretical concepts that will provide some new ways of thinking about the interaction of molecules with metals and the conductance properties of new molecules. We are exploring fabrication schemes that can yield metallic "sockets" with gap spacing in the range 2-20 nm. For example, Figure 6 illustrates 7.5 nm gap in gold electrodes fabricated by shadow evaporation of gold over polystyrene spheres followed by subsequent protection and etching scheme. We are directly measuring conductance and field-modulated conductance in a number of molecular systems including structures such as the one shown above.

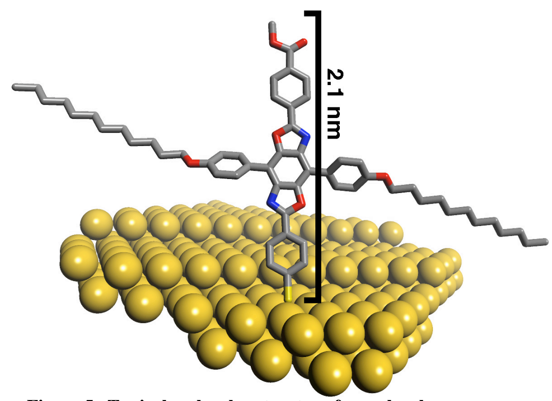

Figure 5. Typical molecular structure for molecular conductance explorations. (Colin Nuckolls)

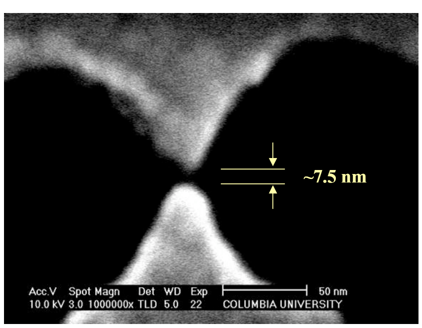

Figure 6. Electron micrograph of 0.7.5 nm gap produced in gold film through non-conventional lithography. (Philip Kim)

References

[1] Further information about this project may be found at the internet web site: www.cise.columbia.edu/nano/ or can be obtained through email to the address: nseccoordinator@www.cise.columbia.edu.
[2] "Engineering Carbon Nanotubes and Nanotube Circuits Using Electrical Breakdown" by P. G. Collins, M. S. Arnold, and Ph. Avouris, Science Vol. 292, p.706 (2001).