Center for Electron Transport in Molecular Nanostructures Columbia University December 16, 2003

Overview.

The Columbia University *Center for Electron Transport in Molecular Nanostructures* was created by Columbia University with National Science Foundation support on September 1, 2001 as one of NSF's Nanoscale Science and Engineering Centers (NSEC). The Nanocenter Team involves 16 members of Columbia University faculty, additional collaborations with faculty from City University of New York, Barnard College and Rowan University, and strong, active collaborations with basic research programs at Lucent Technologies and with IBM Research. The Nanocenter has also received a supporting grant from the State of New York through NYSTAR. The team represents a unique assembly of capabilities in chemical synthesis and chemical manipulation, in fundamental physics of electron dynamics, and in nanoscale device fabrication and characterization. The team also brings strong interaction with an extremely diverse and influential educational community, ranging from K-12 programs in inner-city schools to a wide variety of undergraduate educational activity to graduate and postgraduate research programs with international renown. The Nanocenter seeks to combine these elements into a new and powerful force for the creation of new horizons in nanoscale science.

Goals and directions.

The primary goals of the Columbia Nanocenter are to bring the highest level of fundamental understanding to the fascinating and technologically important phenomena of electron transport from an electron "source" (for example a metal at a defined electric potential) to a "drain" (for example a metal maintained at ground potential) through a single molecule or through molecules assembled on a nanometer scale. These phenomena include conduction: simple movement or motion of electrons through the molecule or the molecular assembly. They also include the capability to control electron conduction within a single molecule or a molecular nanostructure through the application of specified electric field distributions. This latter phenomenon can provide a basis for new paradigms in electronic processing. Thus an ultimate outcome of this program could be the demonstration of a single molecule field effect transistor for example.

Since these are very long-range goals, the Nanocenter has defined specific research directions for investigation that we believe offer the greatest opportunity for attainment of our goals within the specific context of the capabilities and experiences of the Nanocenter members. Our program is built upon strong chemical expertise, particularly in chemical synthesis. It is also built upon profound explorations of the fundamental characteristics of electron transport in materials. Finally it is built upon very close and active collaboration with industrial research laboratories at Lucent Technologies and at IBM Research at Yorktown Heights. The intention is to create a truly cross-disciplinary and highly collaborative research program that is organized as such, rather than to carry out activities through a set of individual research projects.

The Nanocenter, working as a team, has defined three primary research directions for our program that point toward the fundamental needs of the field, but which also provide opportunity for relatively short term needed scientific results. One set of activities are directed toward a *detailed understanding of the growth, structure, and charge transport in nanoscale molecular assemblies* where interesting transport phenomena are expected to exist and which have practical significance. A second set of activities center on *basic understanding of the electronic properties and transport phenomena in carbon nanotube structures and devices based upon them*. We are particularly interested in chemical modification of carbon nanotube structures or device structures and the influence of this modification upon the electron transport properties of these devices. The third set of activities is directed toward the *understanding of electron conductance phenomena in single molecules which are intimately contacted with metallic electrodes*. Here our game plan is fourfold: develop the theoretical picture, synthesize new molecules, fabricate nanoscale "sockets" for the molecules, and characterize through conductance and other measurements. Our intent is to maintain close connection and discussion between these segments and to shift our resource base amongst these segments in order to maximize the overall effectiveness of our program toward its overarching goals.

Structure of the Nanocenter.

Faculty, staff and overall organization. The Columbia Nanocenter is structured around research capabilities and interests of 16 faculty members at Columbia University with additional faculty members from City University of New York (CUNY), Barnard College, and Rowan University. It is also structured to include active collaboration with two research groups at IBM, Yorktown Heights and with two research groups at Lucent Technologies. Overall this program thus encompasses significant participation of approximately 55 people within universities and another 10 or so at Lucent and IBM. The Nanocenter is lead by two scientific directors: Horst Stormer and Ronald Breslow and one managing director, James Yardley. Two additional faculty members, Tony Heinz and George Flynn, join the directors to form the executive committee of the Nanocenter. A program coordinator, Dr. Andrew Levy (75% commitment to NSEC), and an education and outreach coordinator, Alison Biuso (25% commitment to NSEC), assist the leadership in operation of the Nanocenter. The Nanocenter has hired a full time clean room supervisor, Richard Harniman, to help build, maintain, and watch over the fabrication capabilities of the Nanocenter. A special committee chaired by George Flynn oversees our outreach and education program.

We are also able to augment our research activities strategically through invitations to visiting scholars and excellent experienced research scientists. Thus the Nanocenter had in residence for one year Prof. Takao Someya from the University of Tokyo. We have hosted several visitors who have enhanced our intellectual environment including Phil Allen from the physics department at Stony Brook and Peter Feibelman from Sandia. Dr. Shalom Wind, one of the key members of the IBM carbon nanotube and device fabrication teams, is at the Nanocenter for two-year period to help us move forward in molecular conductance measurement. Dr. Mark Hybertsen, an experienced theoretician from Bell Labs and Agere has joined us to strengthen our theoretical efforts. Dr. Latha Venkataraman has also joined the Nanocenter this fall as a research scientist.

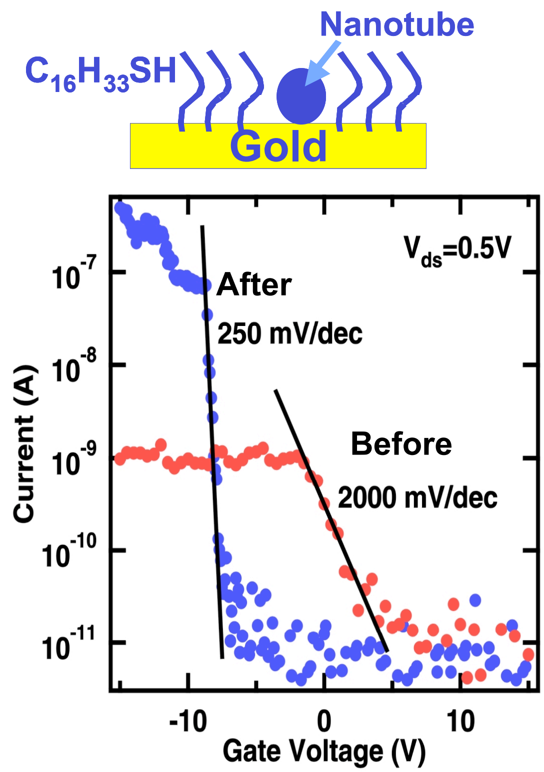
The Nanocenter has appointed an Outside Advisory Board of outstanding and accomplished scientists within the broad scientific community and we are building an Industrial Advisory Board to help us build active and vital interactions with industry beyond the Lucent Technologies and IBM interactions that are at the heart of the program. Columbia University's Center for Integrated Science and Engineering (CISE, formerly the Columbia Radiation Laboratory) oversees the general administration of the program.

Organization of research program. Our policy is to support primarily students or postdocs who are fully devoted to the Nanocenter program in order to assure that all members of the program participate in the overall activities of the Nanocenter. Our research program is structured through three multifunctional and multidisciplinary teams, borrowing from successful industrial research models. The research faculty members operate individually through collaborations and interactions appropriate for the specific research directions chosen. Each team has an identified leader and an identified coordinator who serve to coordinate activity, to convene the teams for scientific discussion, and to encourage interaction and collaboration where appropriate. The team structure and composition changes in congruence with the evolution in the Nanocenter program. In order to facilitate discussion and interaction, we sponsor a cycle of weekly meetings: for each of three sequential weeks, one thrust group meets, typically with one or two highlighted areas for discussion or presentation of recent results. Then for the fourth week in the cycle we hold a Nanocenter-wide graduate student/postdoc seminar, typically with two speakers.

Organization of outreach and education activity. The Outreach and Education Committee has developed a strategic plan for building a strong program coupled to Nanocenter concepts, staff, and capabilities. The plan is built around three basic elements: *Engagement*: "Drawing from and broadening the pool of talented students"; *Growth*: "Involving students in all aspects of our program"; and *Transition*: "Preparation for life after university research in Nanotechnology". The outreach and education coordinator, Alison Biuso, is primarily associated with the undergraduate REU and high school teacher RET programs.

Research accomplishments.

The approach of the Columbia Nanocenter has been to define the overall goals and then to define the best research directions given the scientific capabilities of the center. Thus the Nanocenter has been developing a unique and specific research program. Now, after operation for over 2 years, the Nanocenter program has developed a tremendous amount of momentum and has made a number of significant accomplishments. In exploration of electron transport in carbon nanotubes the team, building on extensive efforts at IBM, has made major progress in defining the importance of the metal-nanotube interface on the characteristics of FET devices. Since the operation of these devices is primarily through electric field modulation of the tunneling of electrons through the Schottky barrier at the nanotube-conductor interface the properties of the devices are critically dependent upon the character of that interface. Thus the group including Prof. Louis Brus and Dr. Xiaodong Cui of Columbia University and Dr. Phaedon Avouris of IBM has discovered that treatment of metal electrodes with simple liquids or gases provides for very precise control of the behavior of these devices. For example, treatment of the interface with a simple solution of an organic molecule can improve the sensitivity of the transistor to applied voltage by a factor of 10.



We have carried out a screening program to explore some of the possibilities for nanotube FET devices for molecular sensing. Alcohols can clearly be sensed with sensitivity and stability, but selectivity remains an open question. In theory we have developed very high quality theoretical capabilities that are letting us explore the electronic properties of short segments and the effects of chemical modification. We have developed new techniques for growing nanotubes that are very useful for device fabrication.

With respect to transport in molecular nanocrystals we have revisited conduction in pentacene and affirmed that mobilities are modest, even at low temperature. We have initiated an exciting basic study of the growth, structure, and conduction properties of single domain pentacene nanocrystals. We have been able to grow such structures one or more monolayers thick and have begun looking at spontaneous charge generation in these systems. We have synthesized a large number of very interesting new molecules which clearly show interesting conduction properties and we are in the process of sorting out the conduction phenomena in these systems. We have also have created molecular systems that assemble into single molecule fibers, or more complex ropes and have begun to examine electric field induced ordering in these systems.

For exploration of the conductance properties of single molecules, we have fabricated metal structures with controlled gap dimensions as small as 4nm using a variety of techniques. We have synthesized a number of very interesting molecules for conduction studies. We have initiated investigation of conductance in a specific molecular system for which the electrode gaps were created through electromigration. We have made significant advances in understanding how to think about a single molecule in contact with a metal.

Outreach and education accomplishments.

Our outreach and education program is moving along very well. Highlights include a short course series including Societal Impacts and Science Policy, Ethical Conduct of Research, Scientific Presentation Skills, and Scientific Writing and Publishing. Other successful programs include an innovative program for high school teachers who work within our laboratories in the summer and maintain interaction throughout the rest of the school year. We also are involved in development of an innovative Engineering Clinic at Rowan University in which students work with professors to utilize engineering principles to enhance the capabilities of the Nanoscience research program.