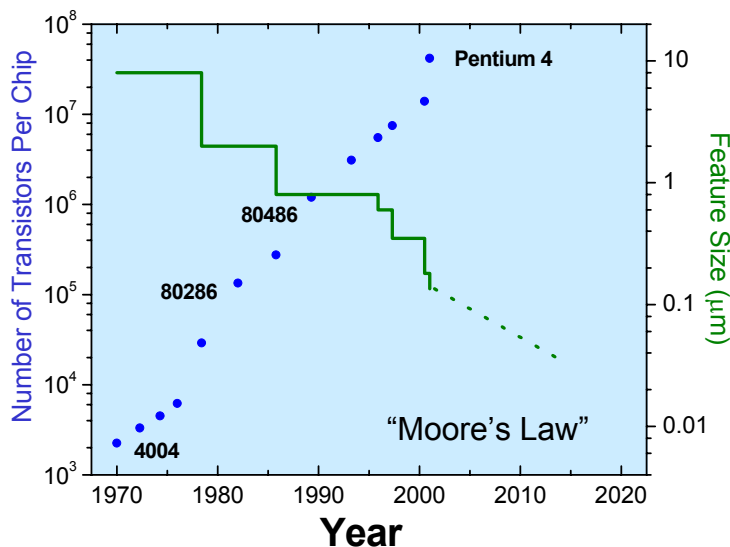
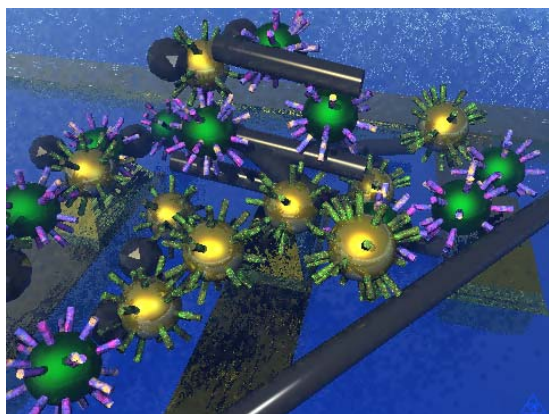
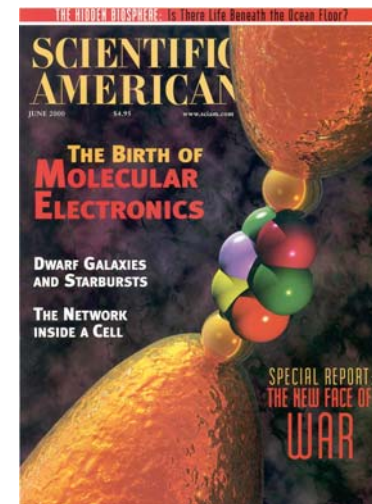


A Presentation to the Visiting Committee on Advanced Technology
 On a New Competence-Building Project in

MOLECULAR ELECTRONICS

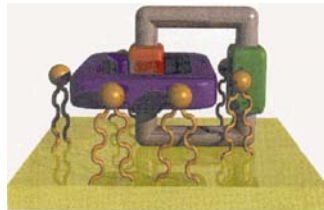
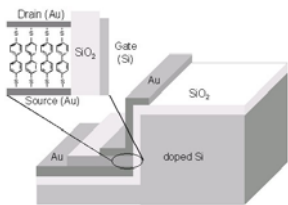


11 December 2001



Molecular Electronics?

- What is “Molecular Electronics?”
- Why now?
- Who are the players?
- How can NIST help?



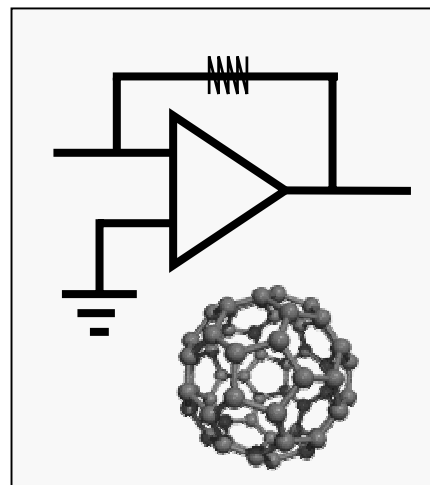
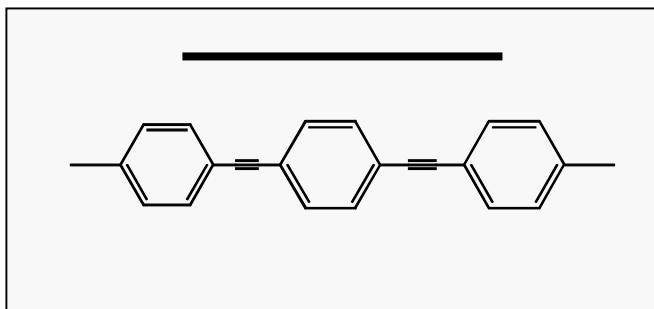
- Our team approach.
- The first year’s progress.
- The road ahead.

Molecular Electronics

— moletronics —

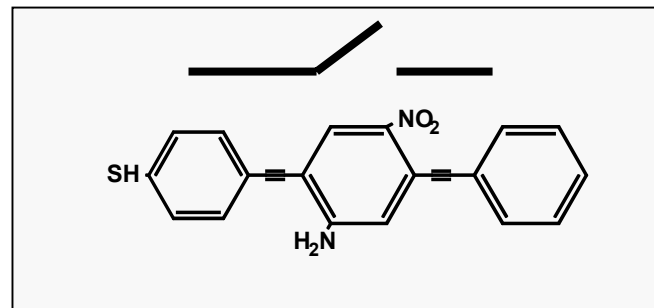
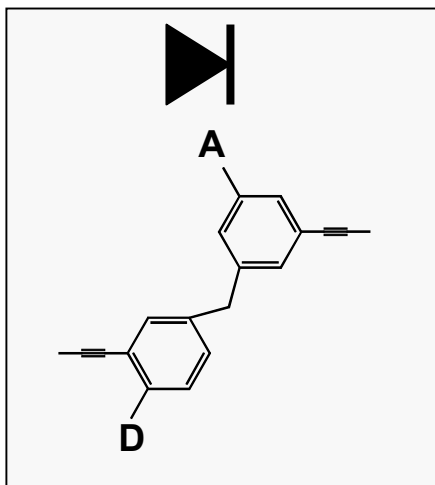
A new technology that uses molecules to perform the function of electronic components.

wire



amplifier

diode



switch

Moletronics in the News

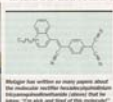
science/technology

TAKING BABY STEPS TO 'MOLETRONICS'

Organic molecules and metallic nanowires are some of the components being eyed for a future nanoscale electronics technology

By Greg Kessler

NIST scientists are taking the first steps toward building a new kind of nanoscale electronics device that will be made from organic molecules and metallic nanowires. They will be made from materials that are easy to process and can be made in large quantities.



Design for a new kind of nanoscale electronics device that will be made from organic molecules and metallic nanowires.

C&E News

news feature

Chemistry meets computing

If individual molecules can be made to process information, they could be the answer to the computer industry's prayers. Philip Dai examines the field of molecular logic, which is at last recording some significant achievements.

Science is heading toward a new era. The development of new tools and techniques in chemistry and physics is leading to a new kind of computing. This new computing is based on the use of individual molecules and nanoscale devices to process information. It is a field that is still in its infancy, but it is showing signs of becoming a major force in the future of computing.



Philip Dai, a scientist at NIST, is shown working in a laboratory setting.

Feature story

Feature story has been being written to cover a wide range of topics in chemistry and physics.

Chemist at NIST, William M. Morehead, is shown working in a laboratory setting.

The first step in the development of a new kind of nanoscale electronics device is to create a device that can process information. This is a field that is still in its infancy, but it is showing signs of becoming a major force in the future of computing.

Nature

The journal Nature is a leading source of information on the latest developments in science and technology.

The journal Nature is a leading source of information on the latest developments in science and technology. It covers a wide range of topics in chemistry and physics, and is widely read by scientists and the general public.

TECHNOLOGY, OCTOBER 18, 2001

NATIONAL NEWS

THE WASHINGTON POST

Scientists Create a Molecular-Scale Transistor

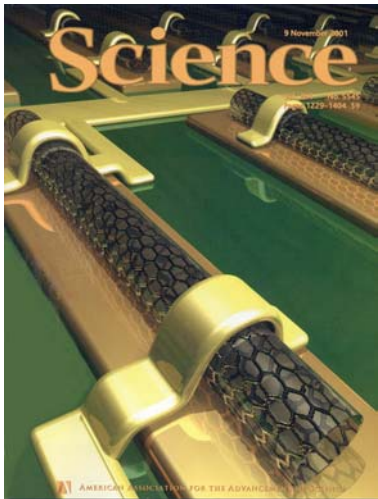
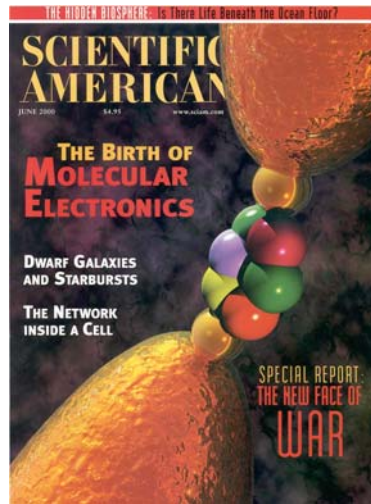
Lucy Technologies Device Is Called Breakthrough in Electronics Miniaturization

By Greg Kessler

WASHINGTON, Oct. 18 (AP) — Scientists have created a transistor that is only a few molecules wide, a breakthrough that could lead to a new generation of tiny electronic devices.

The device, which is only a few molecules wide, is a breakthrough in the field of molecular electronics. It is a device that can be made from organic molecules and metallic nanowires. It is a device that is still in its infancy, but it is showing signs of becoming a major force in the future of computing.

Washington Post



Physics Today

PHYSICS AND THE INFORMATION REVOLUTION

Quantum physics holds the key to the further advance of computing in the postclassical era.

Joel Birbaumer and R. Stanley Williams

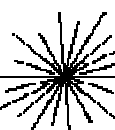
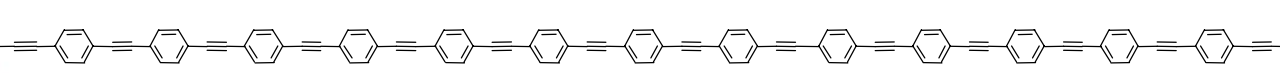
The field of quantum physics is showing signs of becoming a major force in the future of computing. It is a field that is still in its infancy, but it is showing signs of becoming a major force in the future of computing.

PHYSICS AND THE INFORMATION REVOLUTION

Quantum physics holds the key to the further advance of computing in the postclassical era.

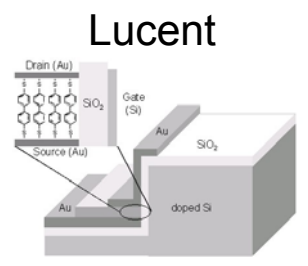
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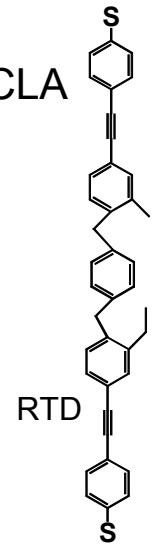
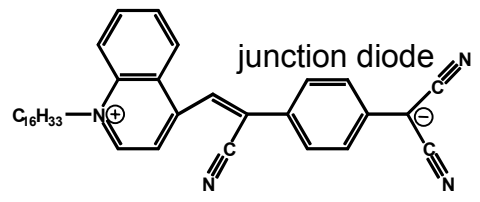
Moletronic Components

Transistors



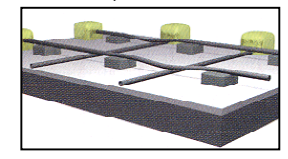
Electrically-Active Molecules

Rice, Univ. of Alabama, UCLA



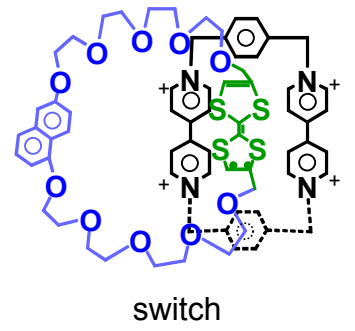
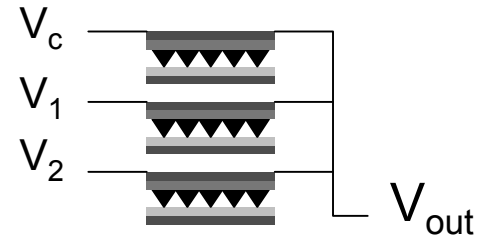
Memory

MEC, Harvard



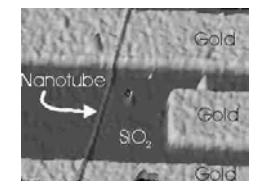
Logic Function

Hewlett-Packard, UCLA, Mitre Corp.



Nanotube FET

IBM

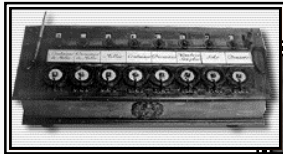


“I was one of the biggest skeptics. Now I believe that this is the inevitable wave of the future.” —R. S. Williams, Hewlett-Packard

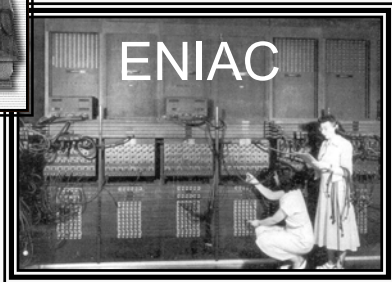
Approaching Fundamental Limits

Computational Paradigm Shifts

1644



1945



ENIAC

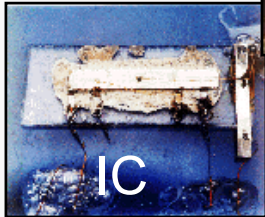


1948



Transistor

1959

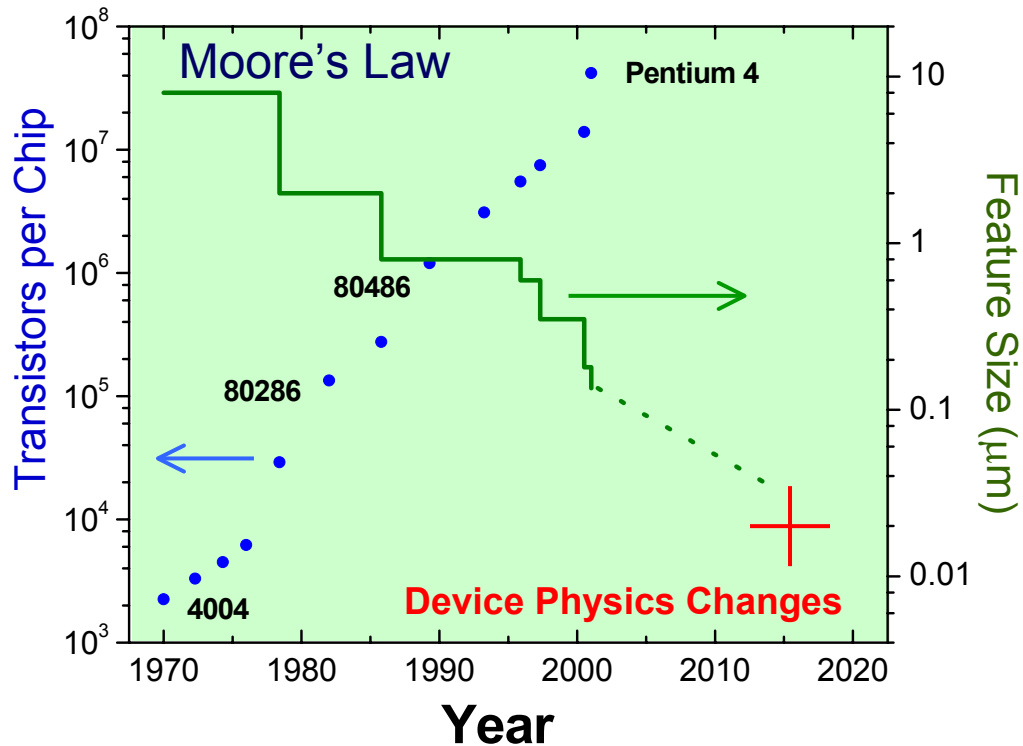


IC

0.013 μm



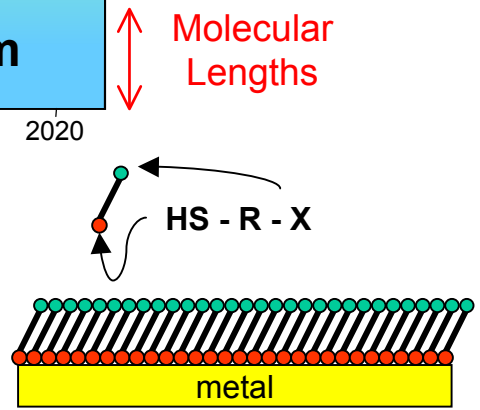
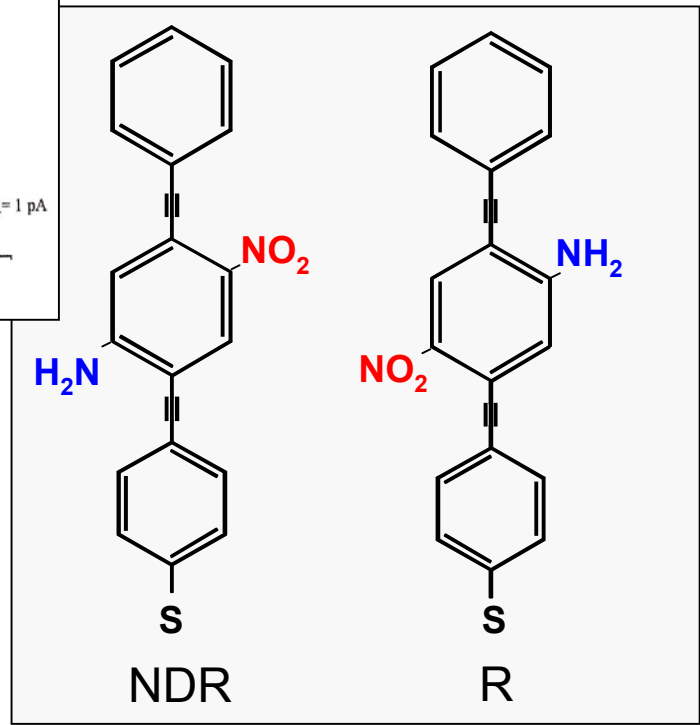
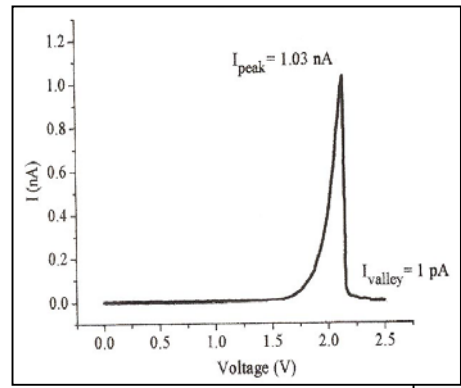
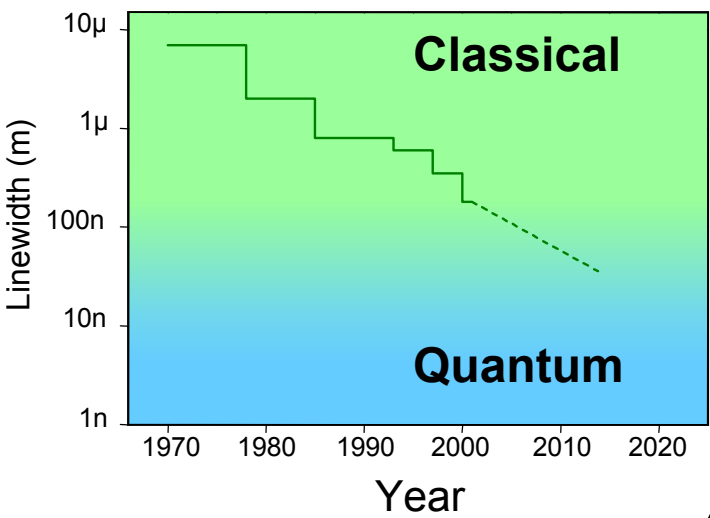
2016



A new components technology is required to maintain the uninterrupted succession of smaller and faster electronic devices.

Why Use Molecules?

- Even big molecules are small.
- Functional control through synthesis.
- Self-assembling devices.



NDR – Negative Differential Resistance
R – Resistor

How Molecules Conduct

Conventional Electronics



insulator

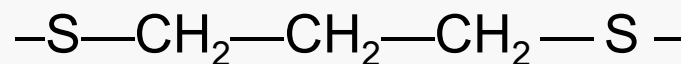


conductor



doped semiconductors

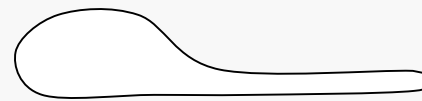
Molecular Electronics



insulator



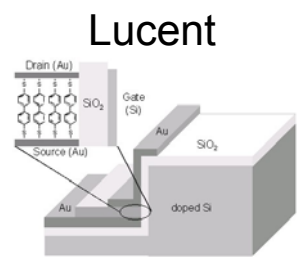
conductor



substituted molecules

Moletronic Components

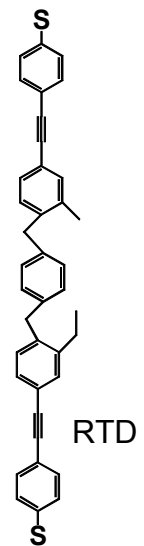
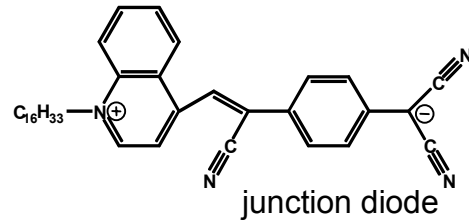
Transistors



Lucent

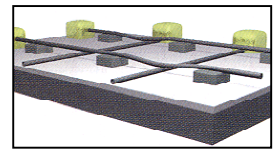
Electrically-Active Molecules

Rice, Univ. of Alabama, UCLA



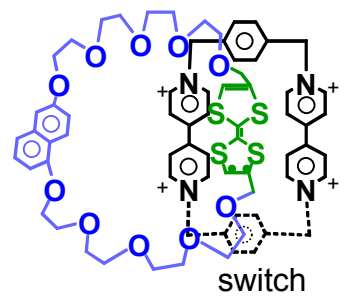
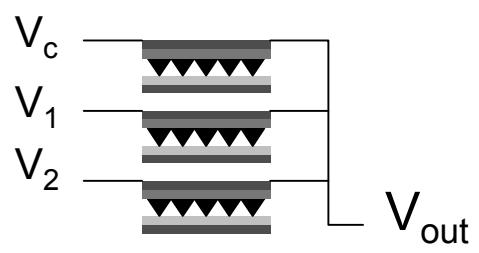
Memory

MEC, Harvard



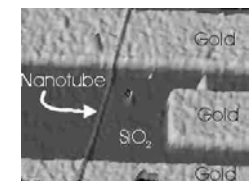
Logic Function

Hewlett-Packard, UCLA, Mitre Corp.

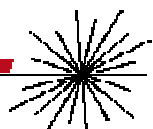


Nanotube FET

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“I was one of the biggest skeptics. Now I believe that this is the inevitable wave of the future.” — R. S. Williams, Hewlett-Packard

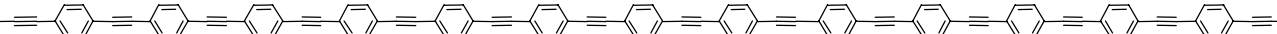


A Role for NIST

To develop the measurement tools and data necessary to measure, model, and control the flow of charge through molecules and ensembles of molecules.

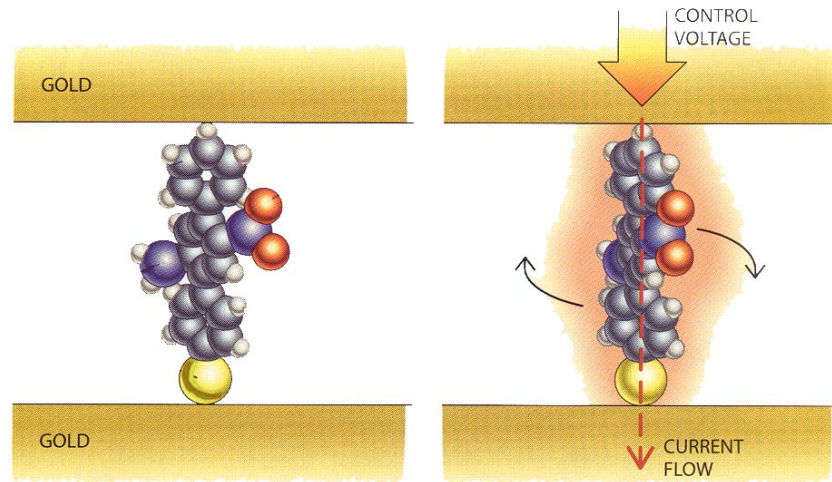
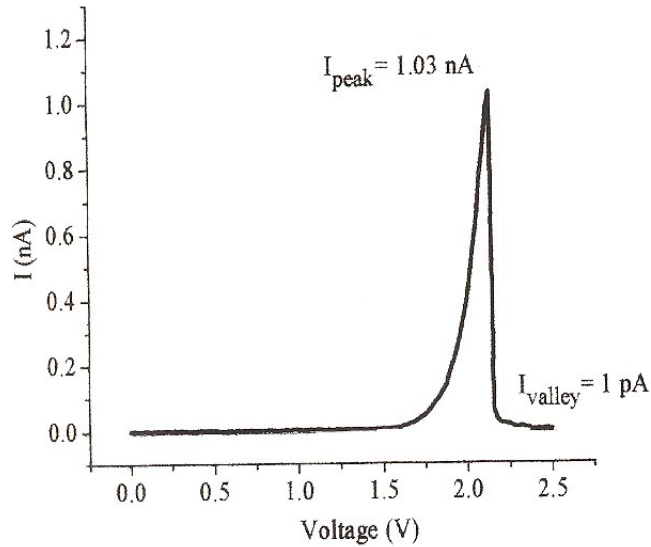
“To knowledge by measurement.”

— Kammerlingh Onnes, Leiden Univ.



Grand Challenges

- Develop Moletronics Metrology
- Correlate Structure and Function

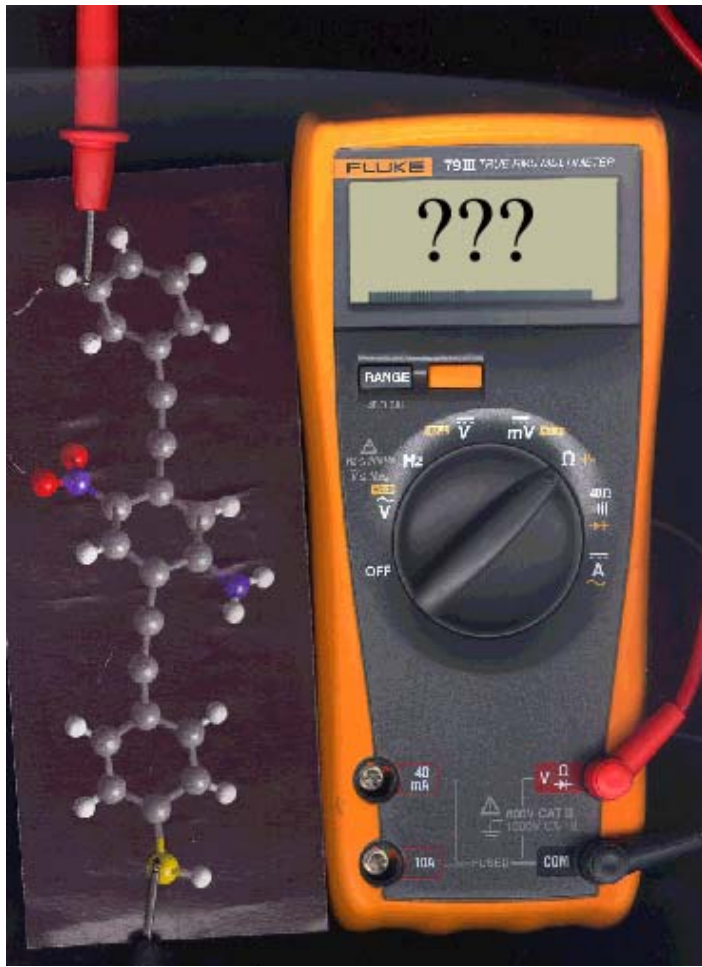


Science, vol. 286, p. 1551
 Sci. Am. June 2000

“The field suffers from an excess of imagination and a deficiency of accomplishment.” —J. Hopfield, Princeton University

Our Role/The Challenge

— What does it mean? How do to make it useful? —

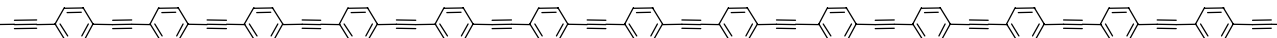


- What is the physical basis for electrical activity in molecular systems?
- How are electrical quantities reliably measured at molecular dimensions?
- What measurements and data are needed to speed this technology to market?

Our Goals

- **To advance the measurement sciences and standards as applied to moletronics.**
 - Quantitative measurement and understanding of molecular conductance
 - Validated models
 - Characterized prototype
 - Test vehicle for molecular components
- **To create a nucleation center for speeding the development of moletronics technology.**

“New directions in science are launched by new tools much more often than by new concepts.” — Dudley Herschbach, Harvard Univ.



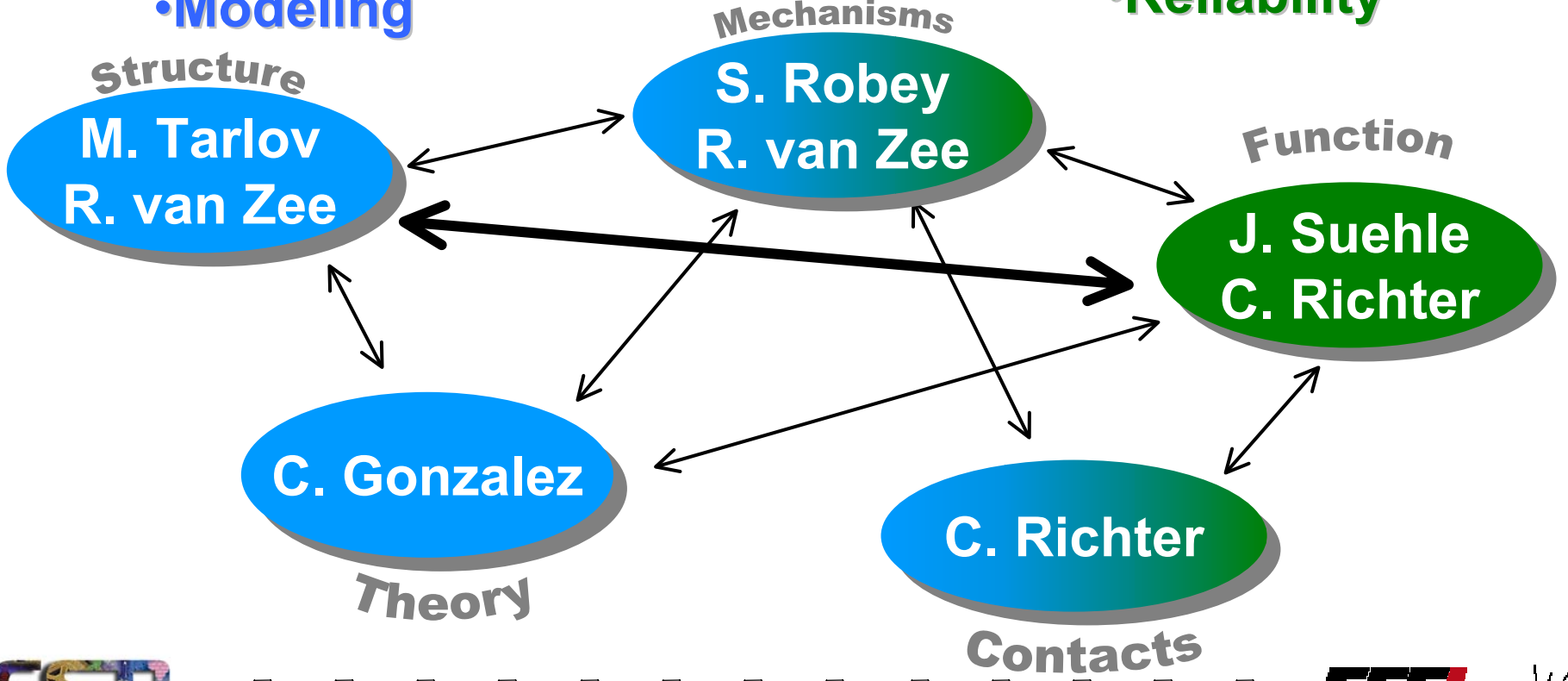
A Multidisciplinary Effort

Chemistry

- Self-Assembly
- Structure
- Mechanisms
- Modeling

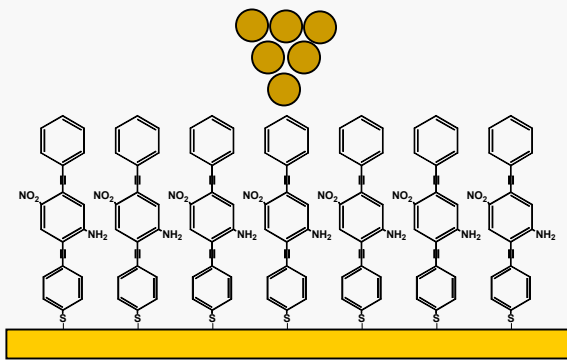
Electrical Engineering

- Contacts
- Integration
- Performance
- Reliability

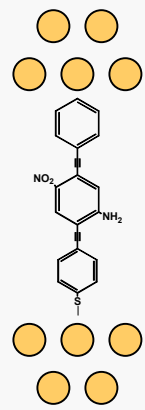
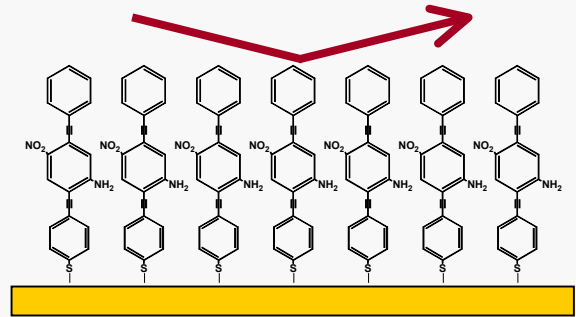


Research Emphases

Electrical Properties of Small Ensembles

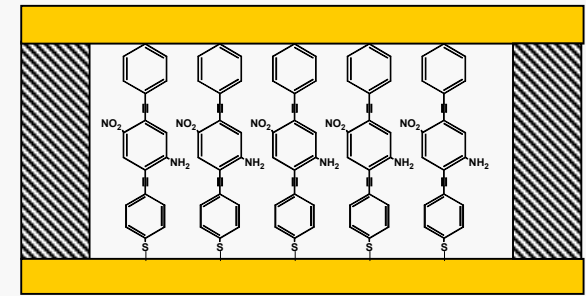


Structure of Electrically-Active, Molecular Films



$$g(E) = \frac{2e^2 T^2}{\pi \hbar \gamma^2} \Delta_D \Delta_A$$

Theory

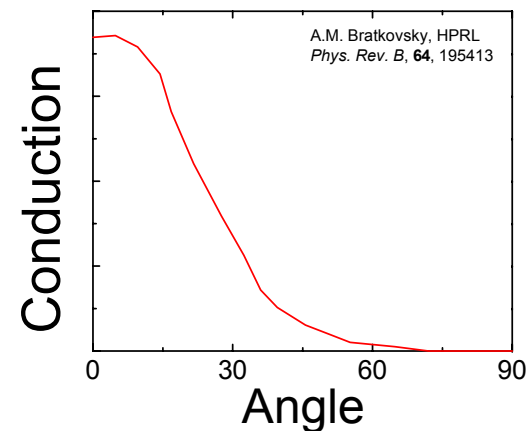
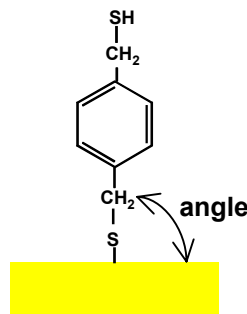
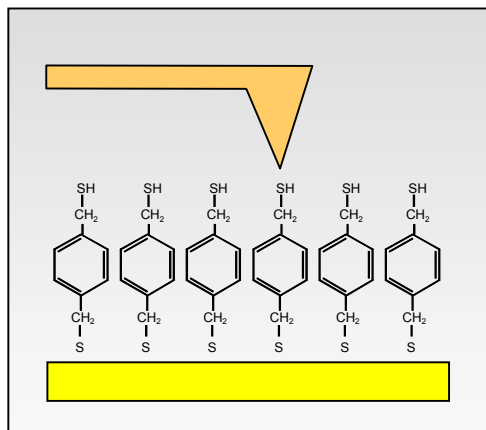
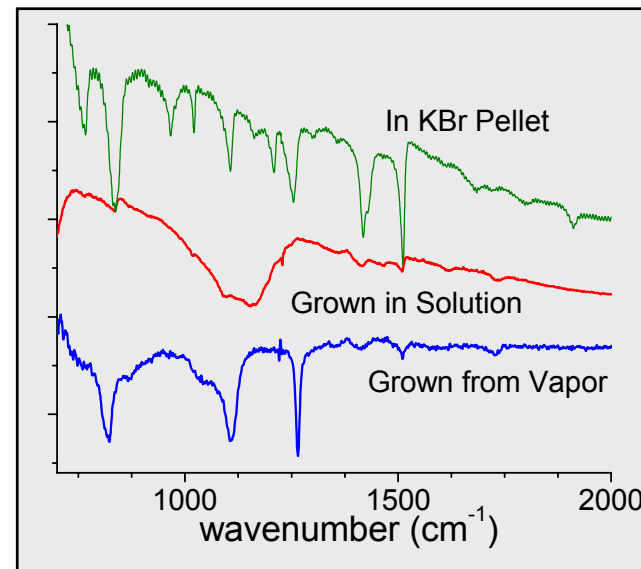
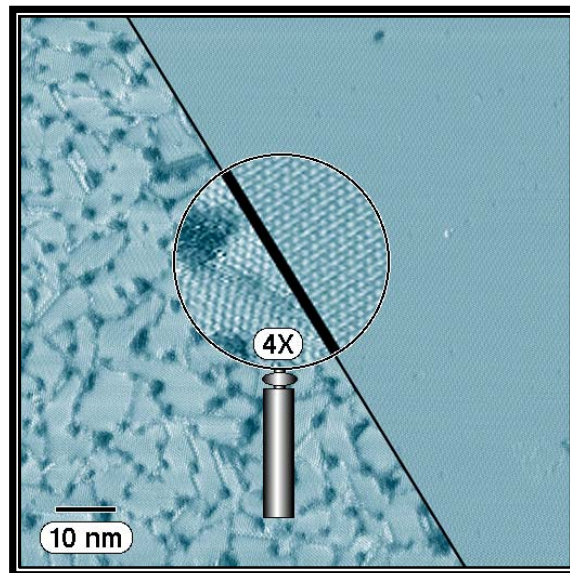
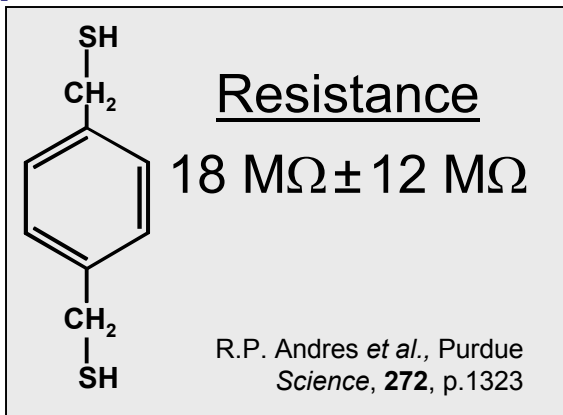


Electrical Properties of Large Ensembles

Resistance of Small Ensembles

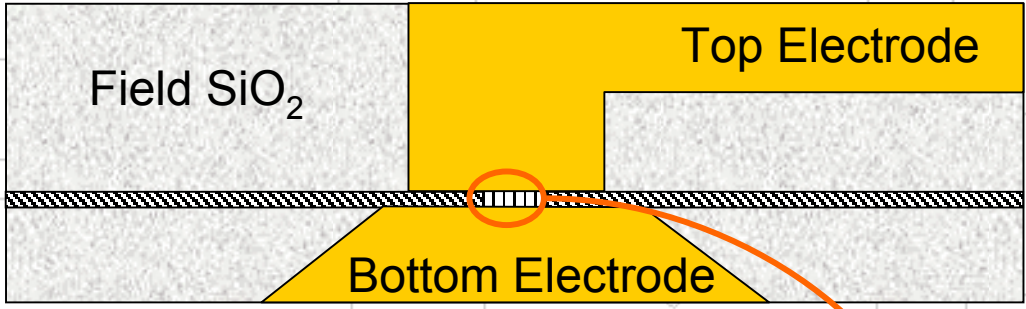
- Studying Film Structure -

p-benzenedimethanethiol

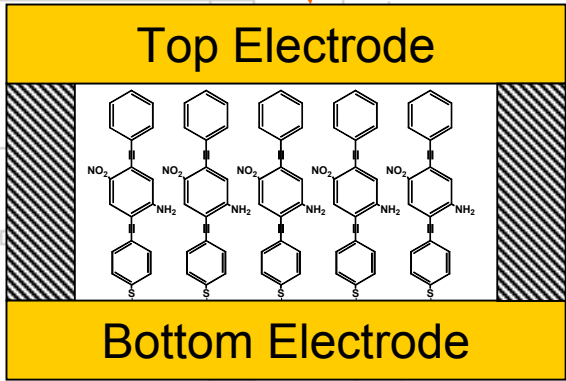
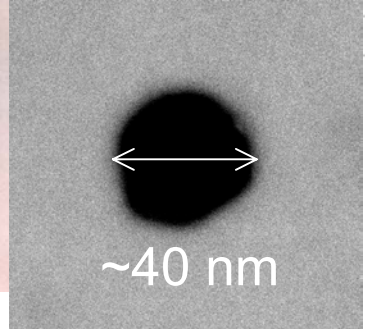
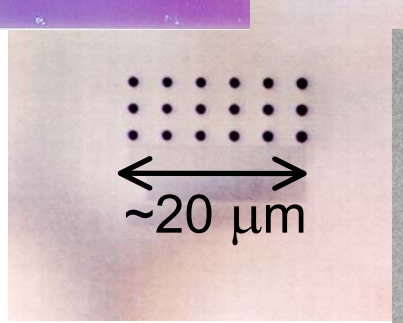
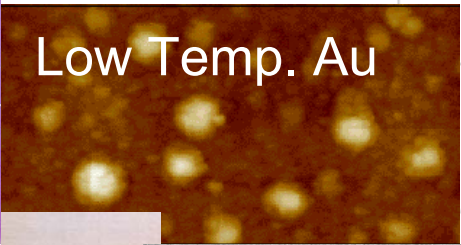


From Molecules to Devices

- Building Test Structures -



Ultra-thin SiO₂
2 nm - 10 nm

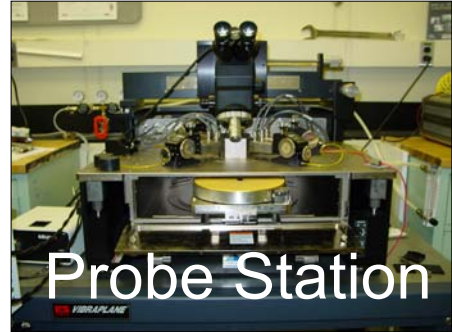
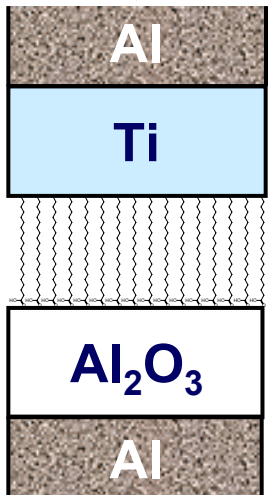
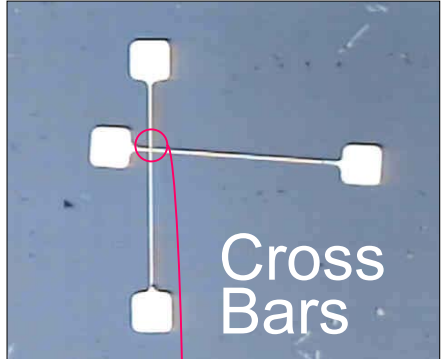


Molecular Length
(2 nm - 10 nm)

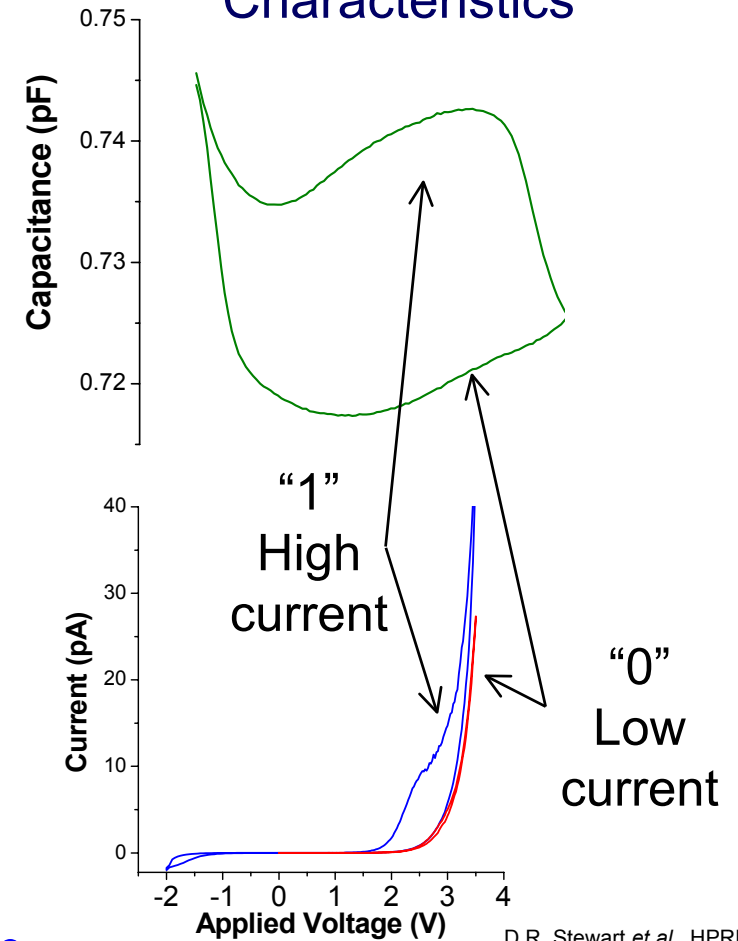
No. of Molecules
(10 nm - 100 nm)

Testing Device Performance

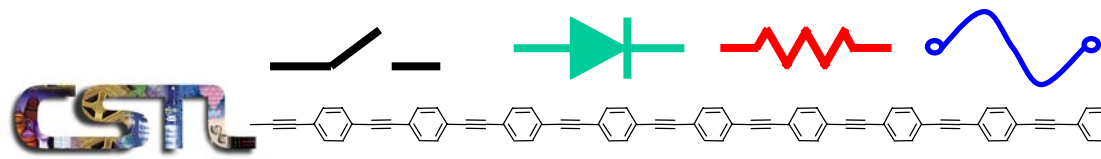
- Reliable Electrical Measurements -



Device Operating Characteristics



D.R. Stewart *et al.*, HPRL
Bull. Am. Phys. Soc., 46, p.1



Modeling Molecular Switches

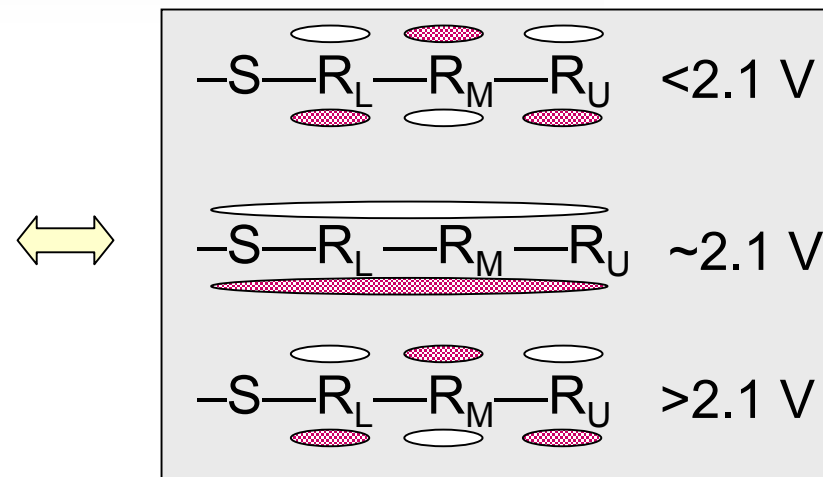
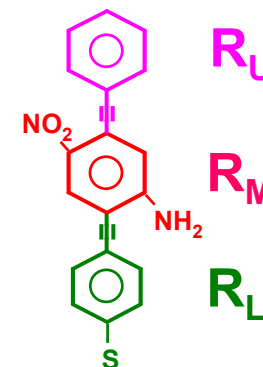
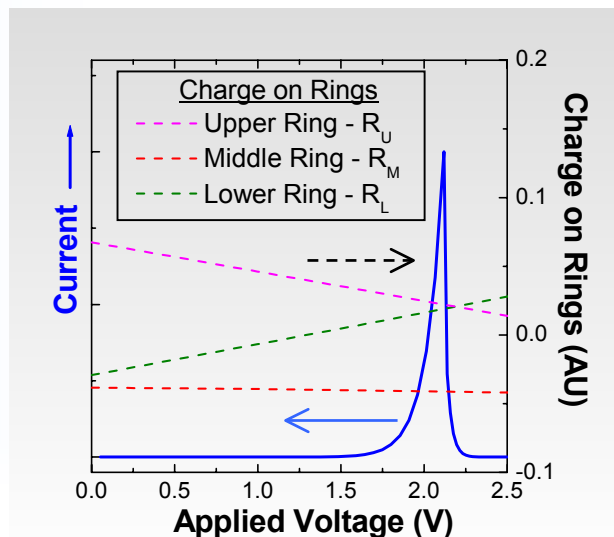
- Understanding Electrical Function and Molecular Structure -

Kohn-Sham Equations

$$F[p(r)] = E_{hf}[p(r)] + E_x[p(r)]$$

$$\{T + V_{hf}(r) + V_n(r) + V_x(r)\} \varphi_i = \varepsilon \varphi_i$$

- Significant charge density localization at voltages below 2.1 V (no current).
- Near 2.1 V maximum de-localization of charge density (maximum current).
- Above 2.1 V charge density localization occurs again (no current).



The Road Ahead

- **Small Ensemble Conduction Experiments**



- **Test Structure Assessment**

- **Electronic Structure Characterization**



- **Conduction Modeling**

Leveraging our Resources

• Nanocell Molecular Computer Collaboratory (Molecules, Electrical Characterization)

- J. M. Tour, Rice University
- M.A. Reed, Yale University
- P.S. Weiss, Penn State University



• Hewlett-Packard Research Labs (Devices, Electronic Structure)

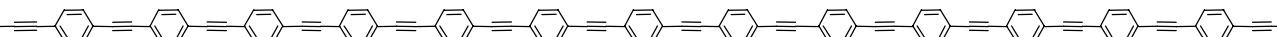
- R.S. Williams
- P.J. Kuekes



i n v e n t

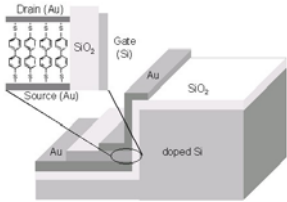
• Naval Research Laboratory (Molecules)

- R. Shashidhar

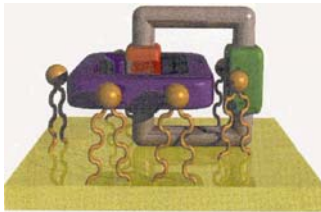


Molecular Electronics!

- Important Technology
 - Revolutionary
 - Timely
 - Critical Role for NIST



- Interdisciplinary Team
- Strong Partnerships with Industry & Universities



Strategies for Success