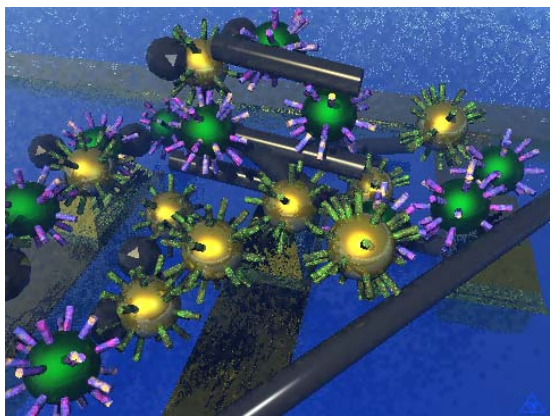
NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

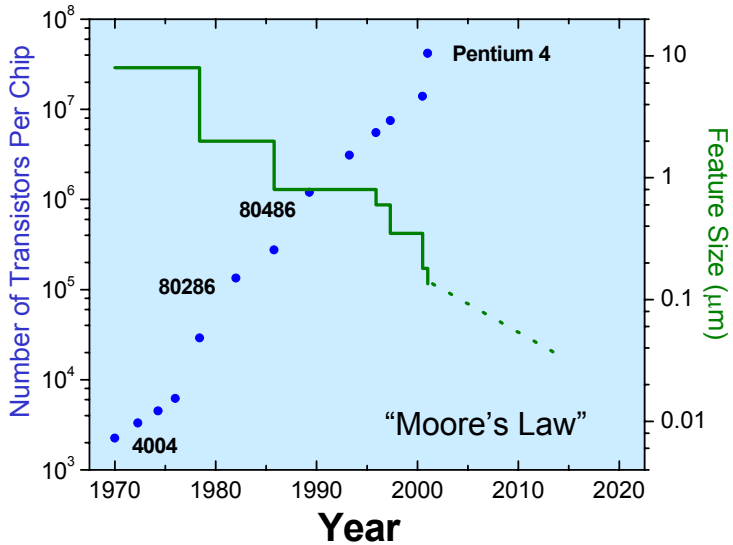
NIST CENTENNIAL 1901-2001

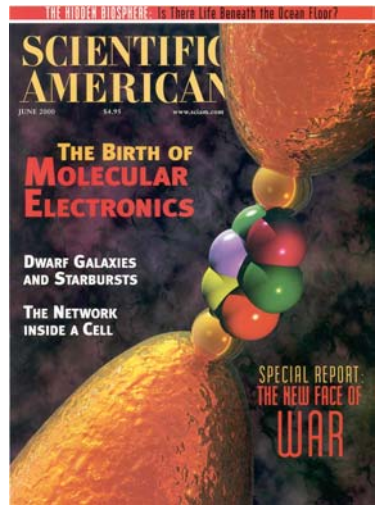
A Presentation to the Visiting Committee on Advanced Technology

On a New Competence-Building Project in

MOLECULAR ELECTRONICS



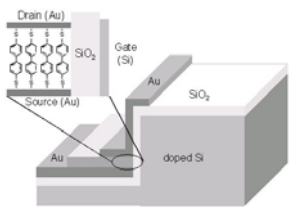


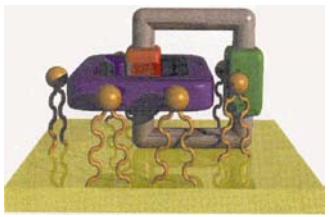


11 December 2001

Molecular Electronics?

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





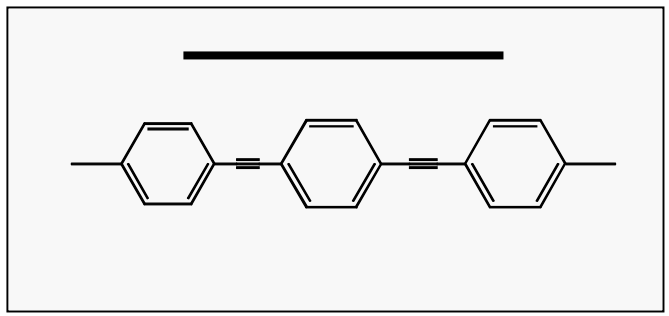
- Our team approach.
- The first year's progress.
- The road ahead.

Molecular Electronics

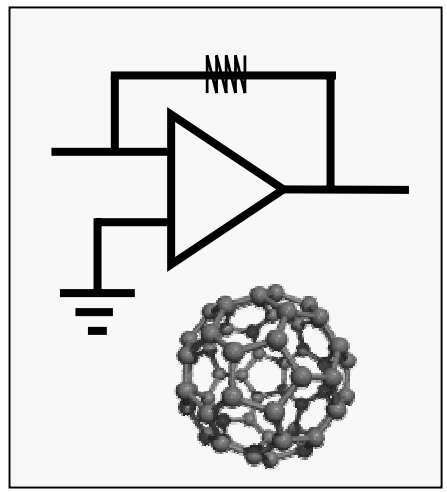
— moletronics —

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

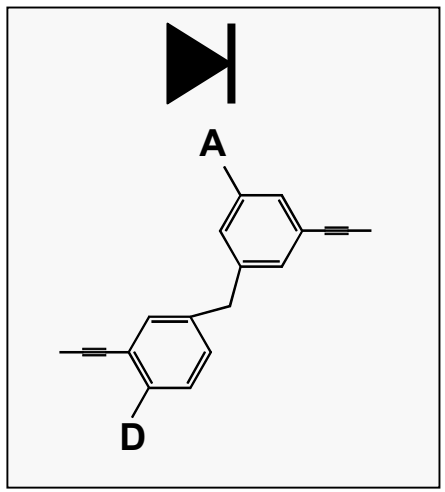
wire



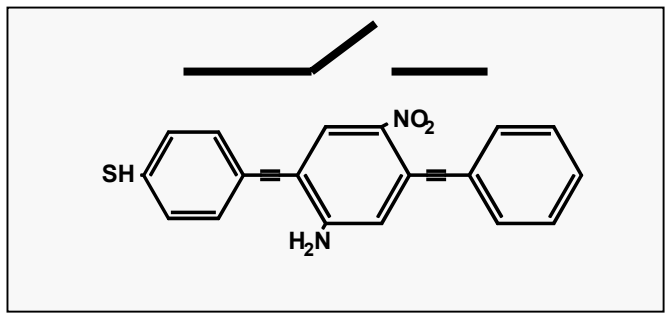
amplifier



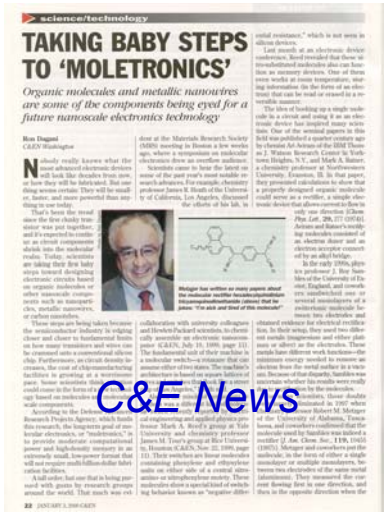
diode



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

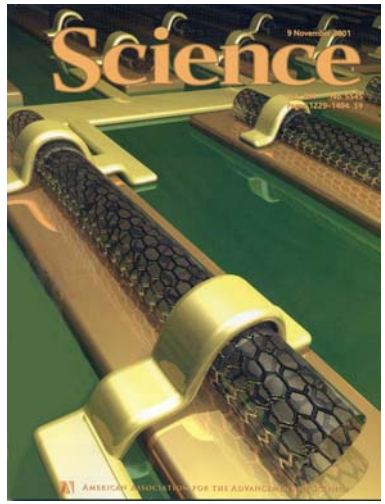
C&E News


THURSDAY, OCTOBER 18, 2001 — NATIONAL NEWS — THE WASHINGTON POST

Scientists Create a Molecular-Scale Transistor

Lucent Technologies Device Is Called Breakthrough in Electronics Miniaturization

Washington Post

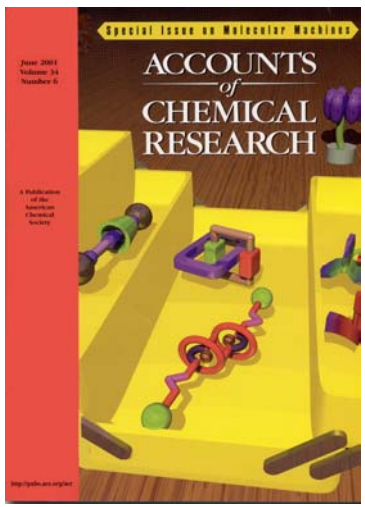


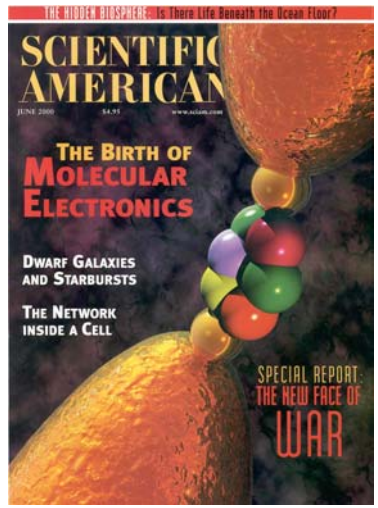

news feature

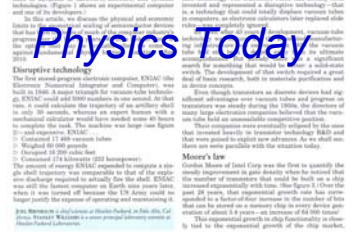
Chemistry meets computing

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

Nature





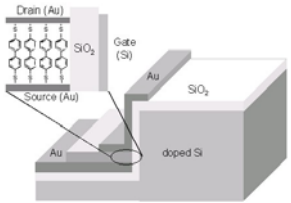

PHYSICS AND THE INFORMATION REVOLUTION

Physics Today

Moletronic Components

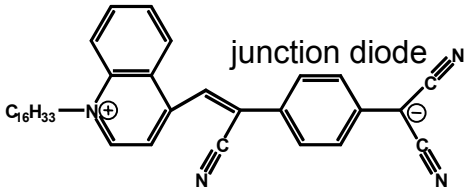
Transistors

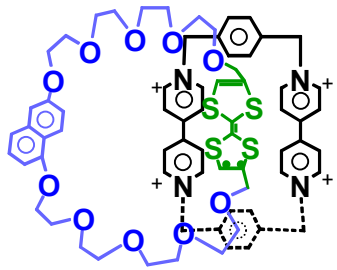
Lucent



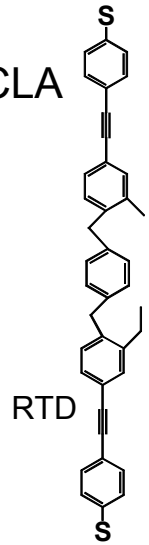
Electrically-Active Molecules

Rice, Univ. of Alabama, UCLA



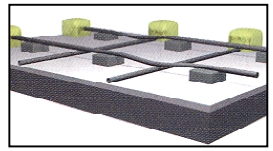


switch



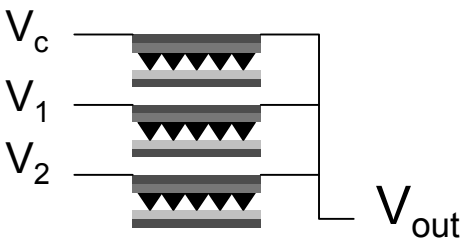
Memory

MEC, Harvard



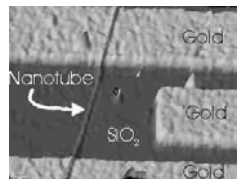
Logic Function

Hewlett-Packard, UCLA, Mitre Corp.



Nanotube FET

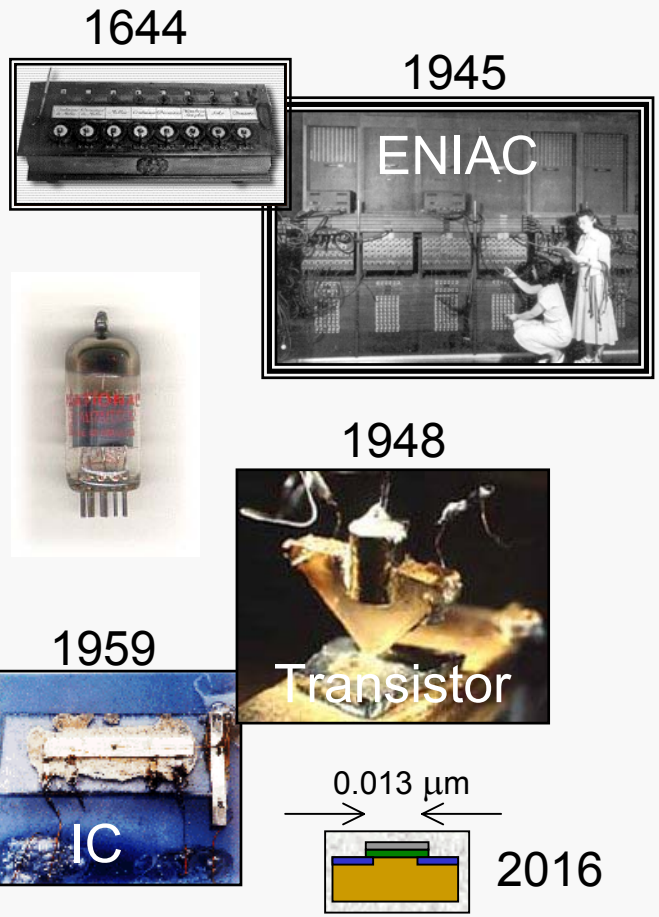
IBM

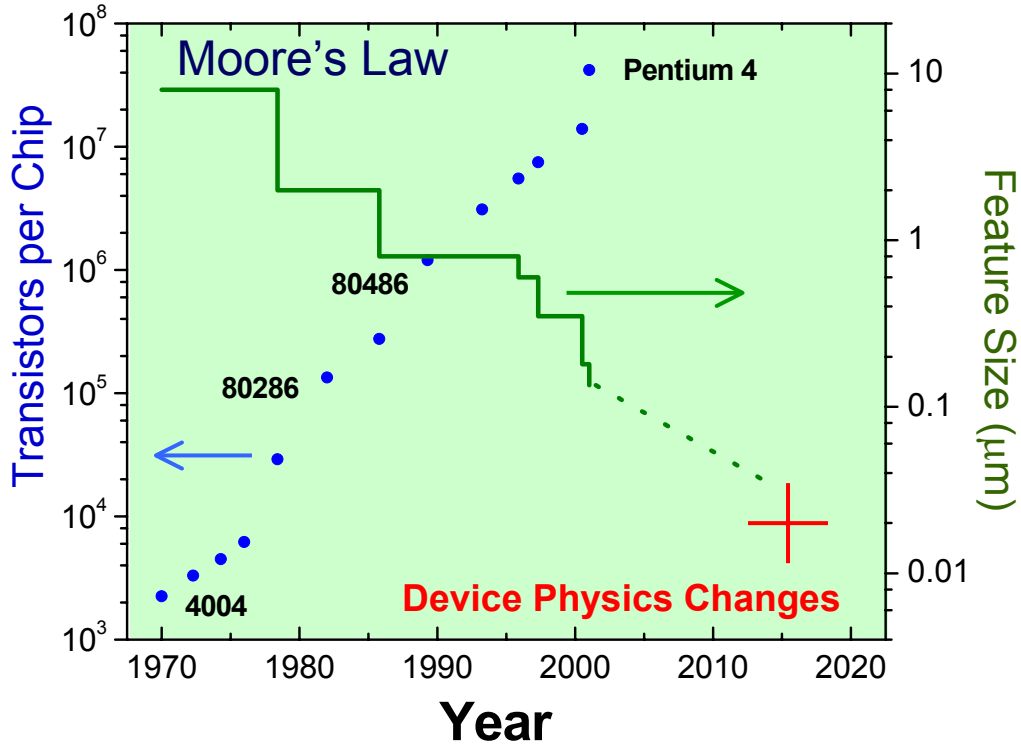


"I was one of the biggest skeptics. Now I believe that this is the inevitable wave of the future." —R. S. Williams, Hewlett-Packard

Approaching Fundamental Limits

Computational Paradigm Shifts

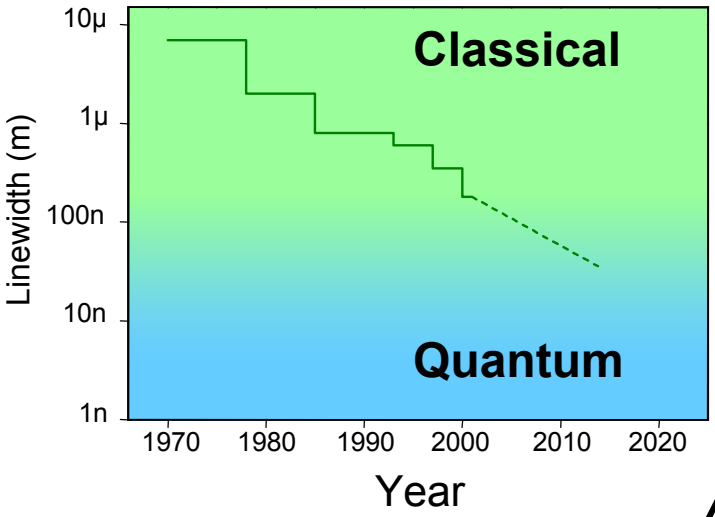




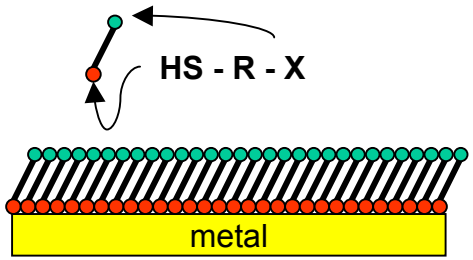
A new components technology is required to maintain the uninterrupted succession of smaller and faster electronic devices.

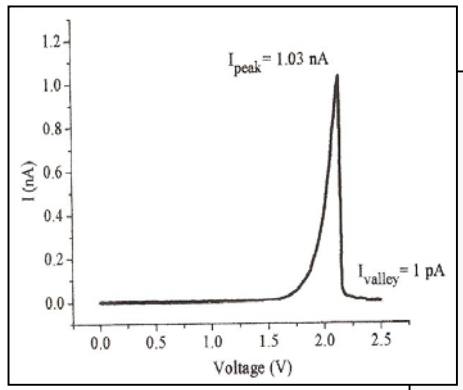
Why Use Molecules?

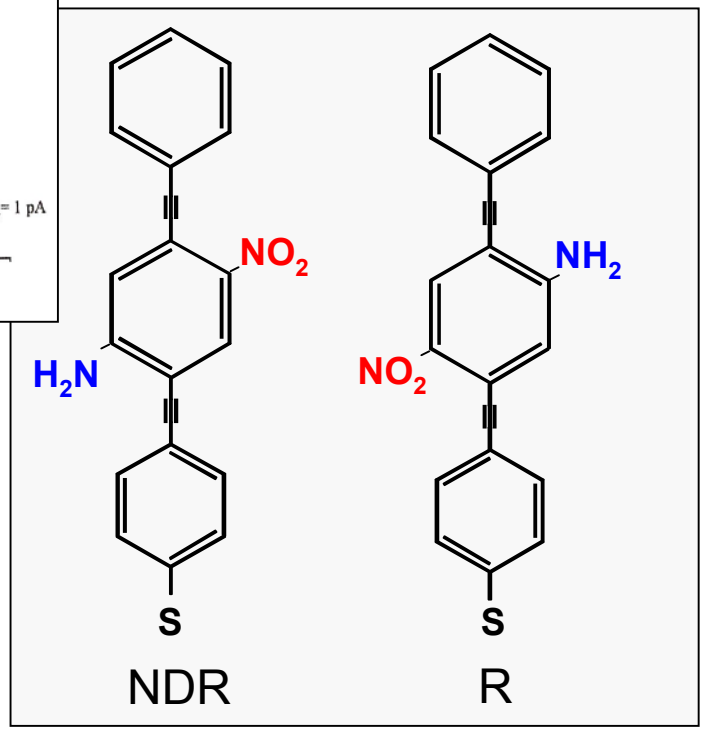
- Even big molecules are small.
- Functional control through synthesis.
- Self-assembling devices.



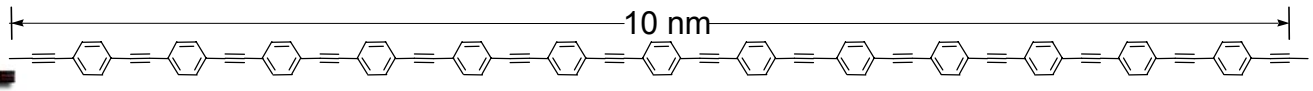
Molecular Lengths







NDR – Negative Differential Resistance
R – Resistor



How Molecules Conduct

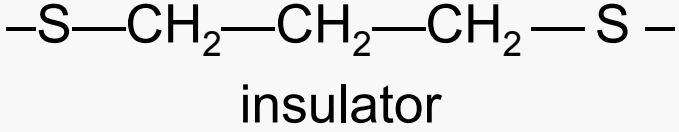
Conventional Electronics

insulator

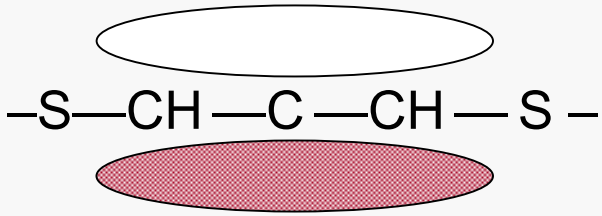
conductor

doped semiconductors

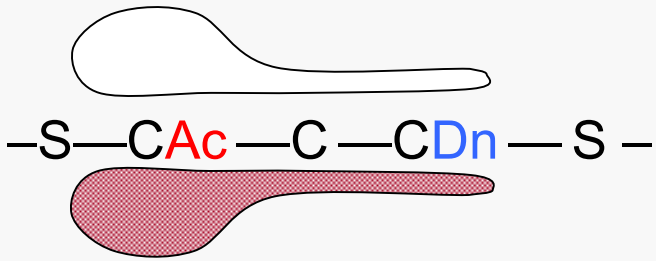
Molecular Electronics



insulator



conductor

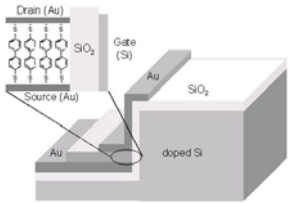


substituted molecules

Moletronic Components

Transistors

Lucent



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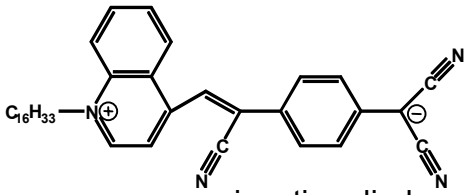
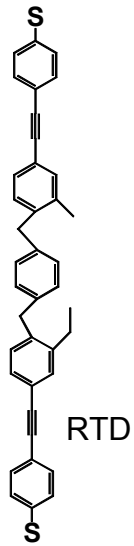


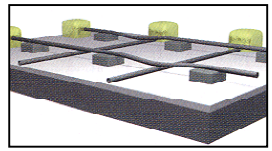
junction diode



RTD

Memory

MEC, Harvard



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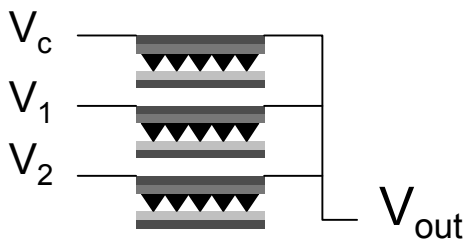
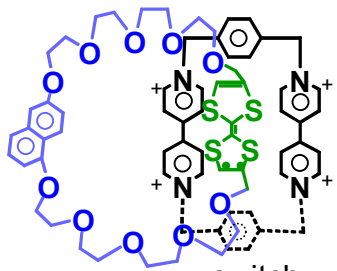
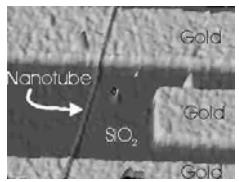




switch

Nanotube FET

IBM



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A Role for NIST

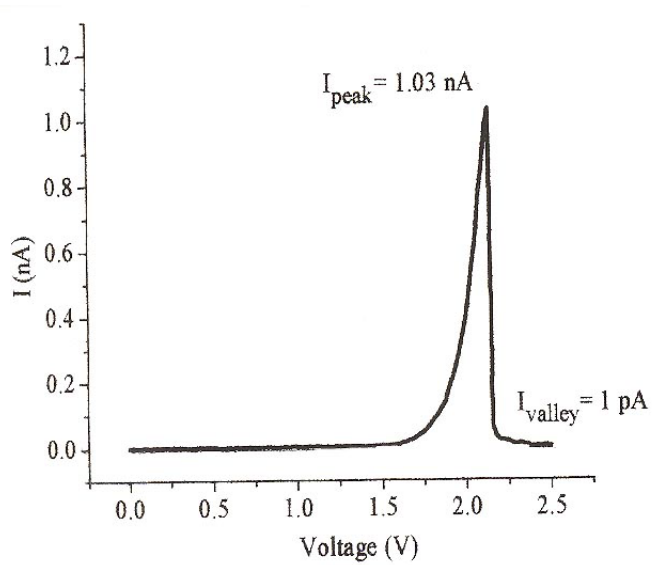
To develop the measurement tools and data necessary to measure, model, and control the flow of charge through molecules and ensembles of molecules.

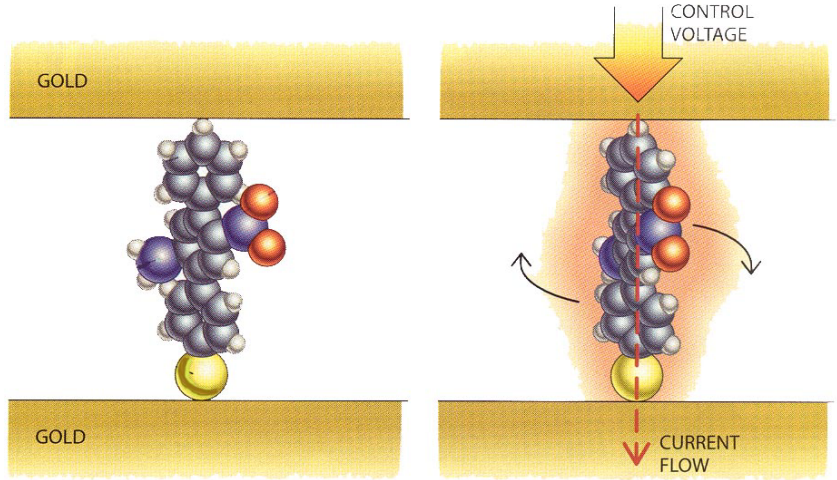
"To knowledge by measurement."

— 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 moletronic 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**

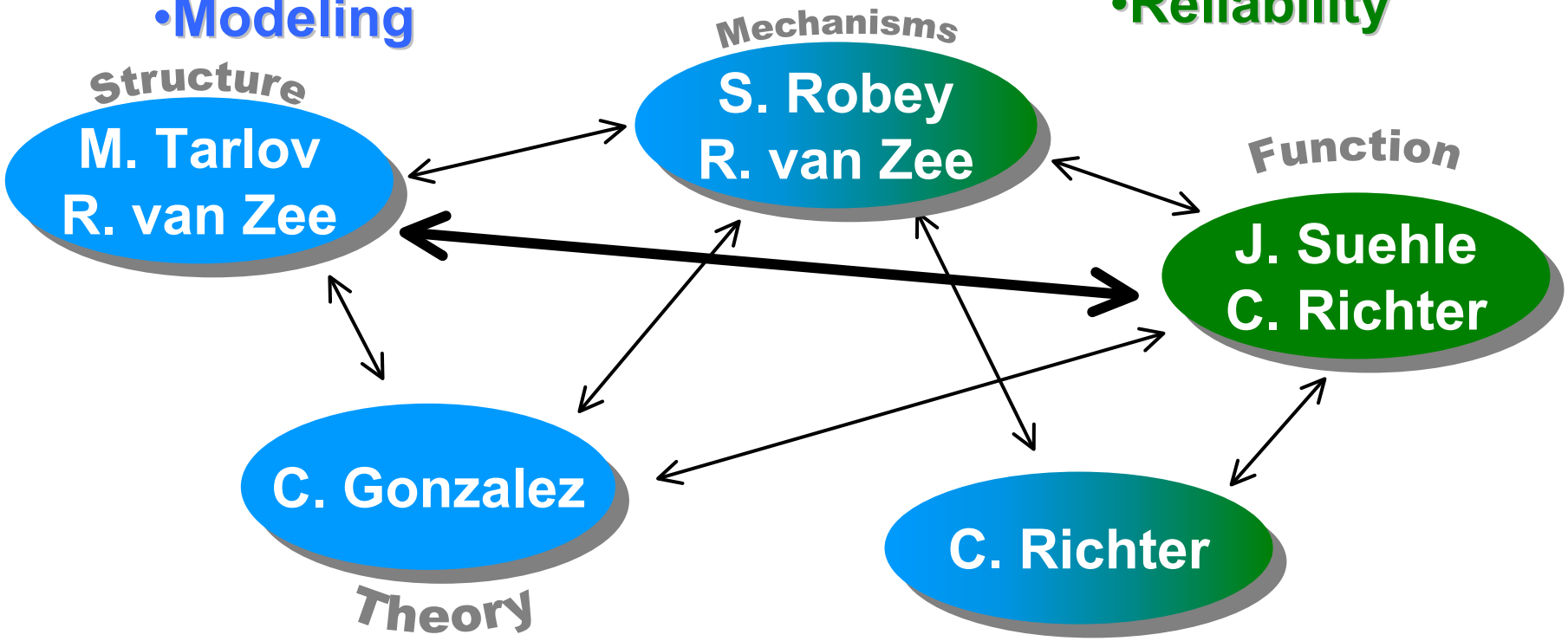
- **To create a nucleation center for speeding the development of moletronics technology.**

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

A Multidisciplinary Effort

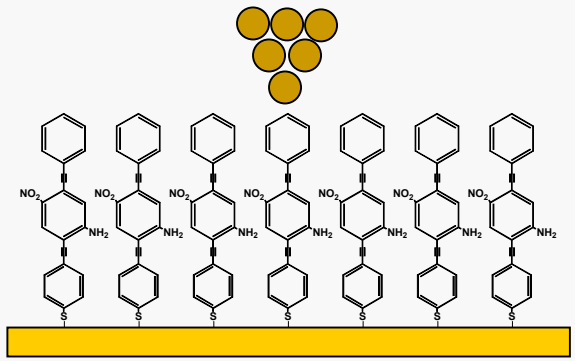
Chemistry
- Self-Assembly
- Structure
- Mechanisms
- Modeling

Electrical Engineering
- Contacts
- Integration
- Performance
- Reliability

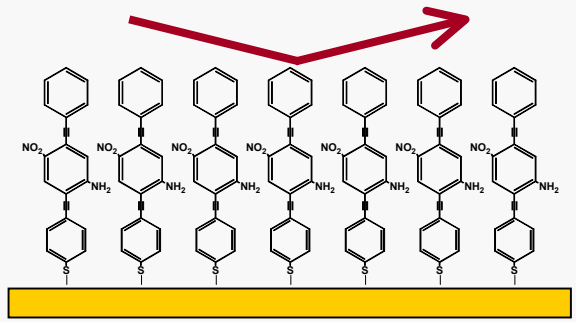


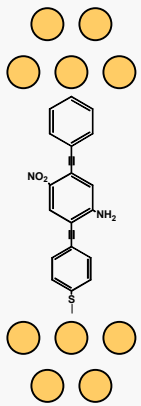
Research Emphases

Electrical Properties of Small Ensembles



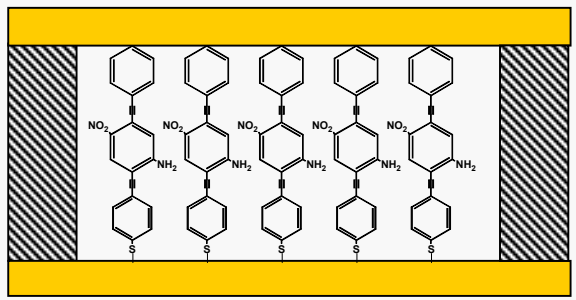
Structure of Electrically-Active, Molecular Films





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

Theory

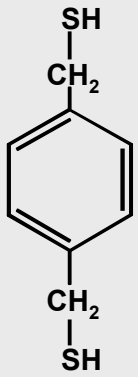


Electrical Properties of Large Ensembles

Resistance of Small Ensembles

- Studying Film Structure -

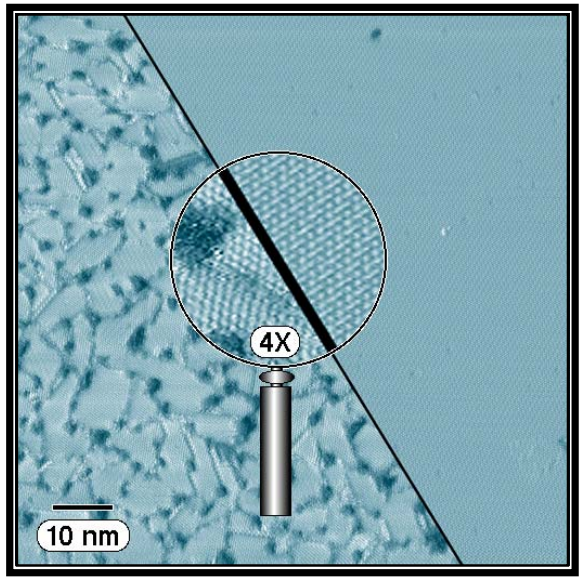
p-benzenedimethanethiol

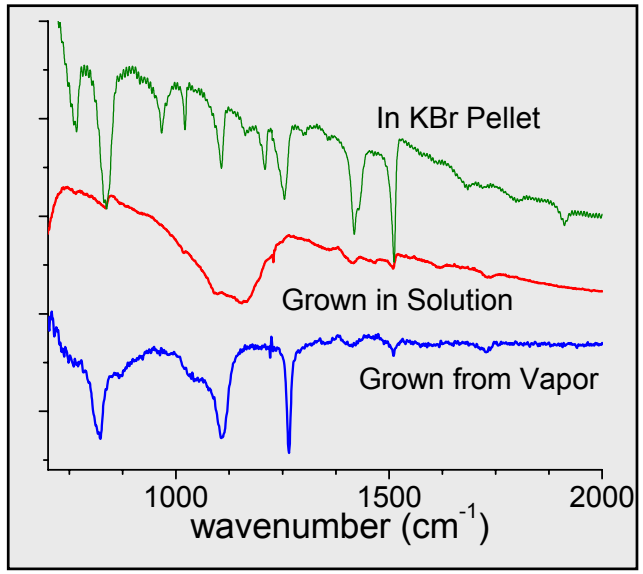


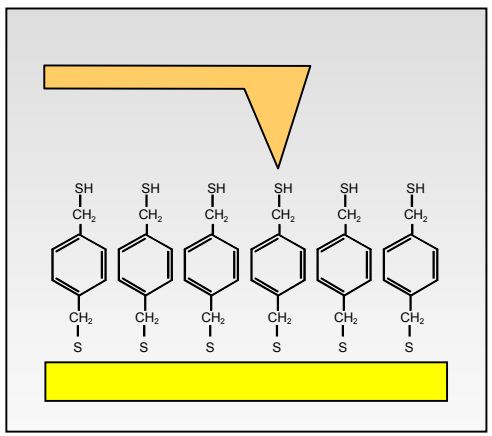
Resistance

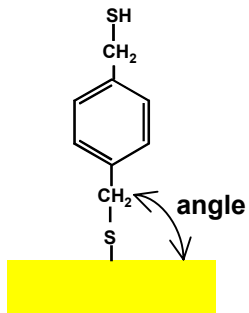
18 MΩ ± 12 MΩ

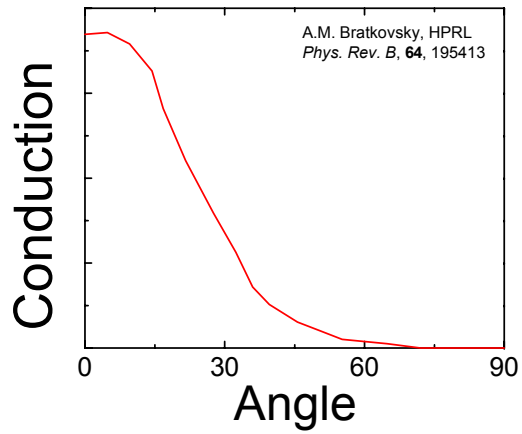
R.P. Andres *et al.*, Purdue
Science, **272**, p.1323





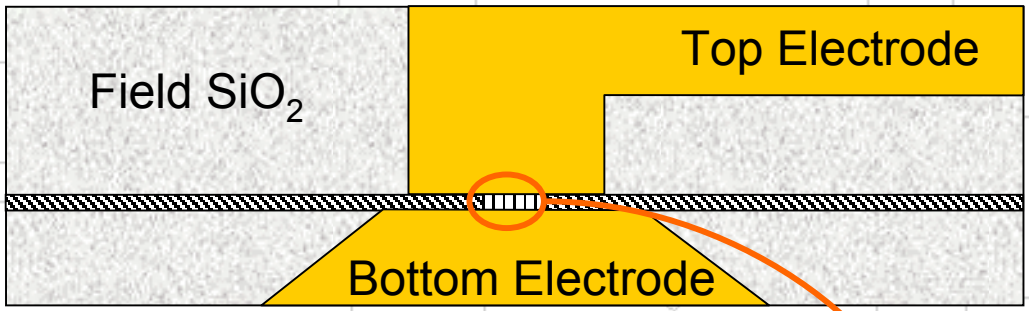




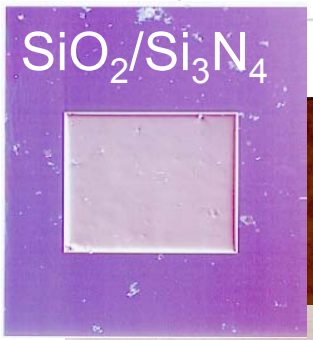


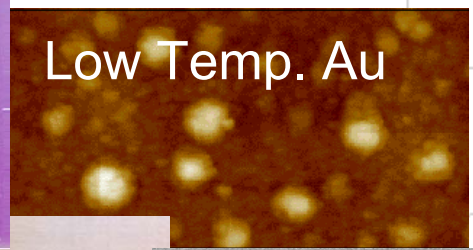
From Molecules to Devices

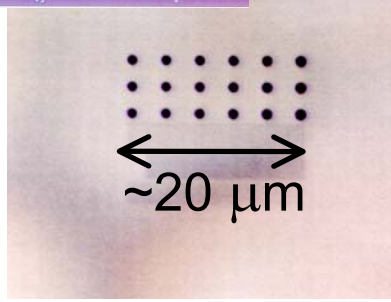
- Building Test Structures -

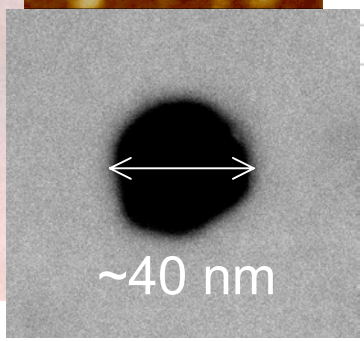


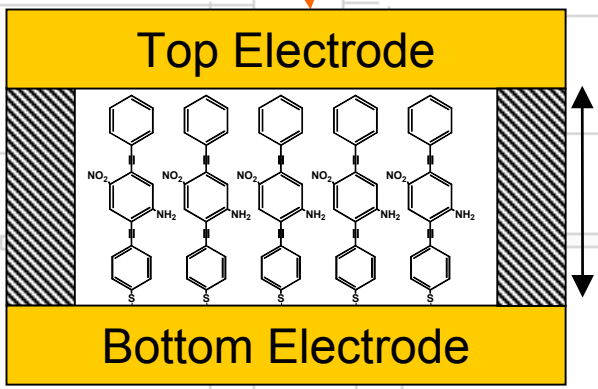
← Ultra-thin SiO_2
2 nm - 10 nm









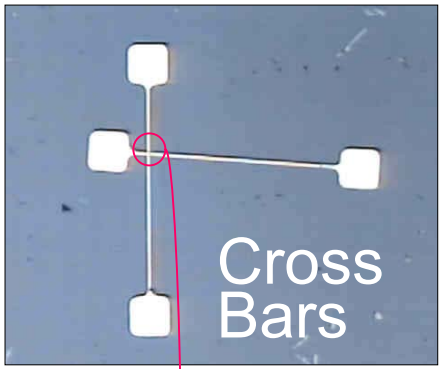


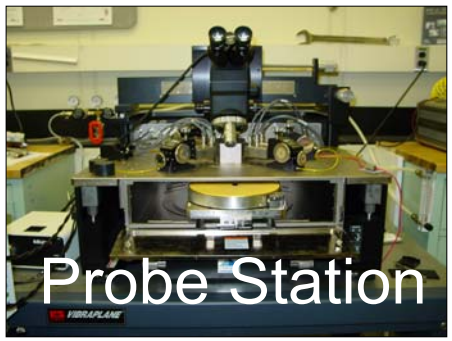
Molecular Length
(2 nm – 10 nm)

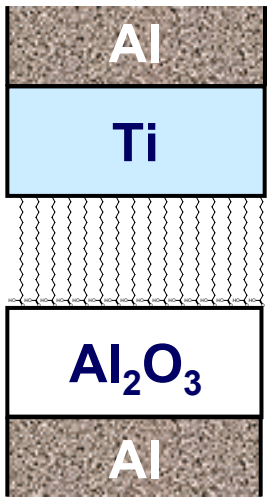
No. of Molecules
(10 nm - 100 nm)

Testing Device Performance

- Reliable Electrical Measurements -

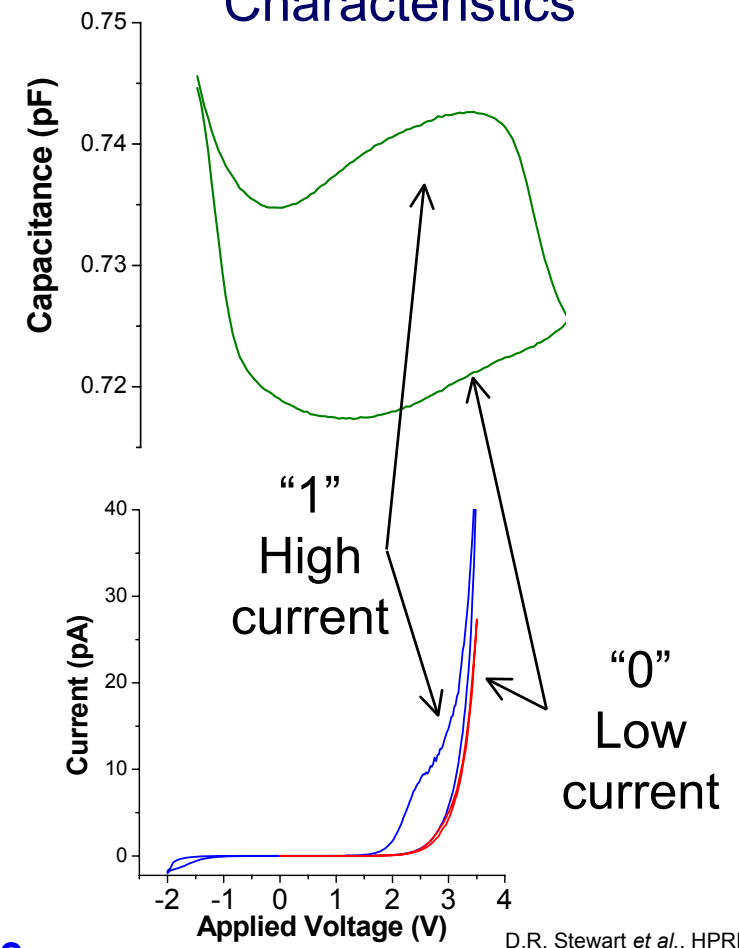






$CH_3(CH_2)_{18}CO_2H$

Device Operating Characteristics



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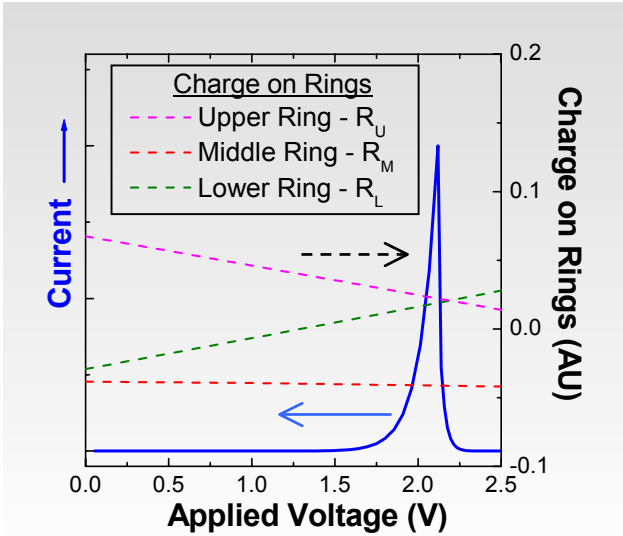
Modeling Molecular Switches

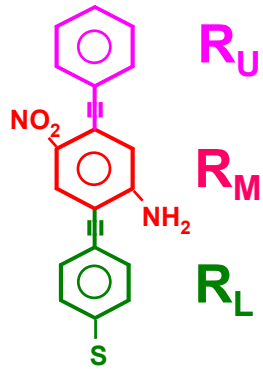
- Understanding Electrical Function and Molecular Structure -

Kohn-Sham Equations

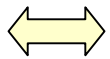
$$F[p(r)] = E_{hf}[p(r)] + E_x[p(r)]$$

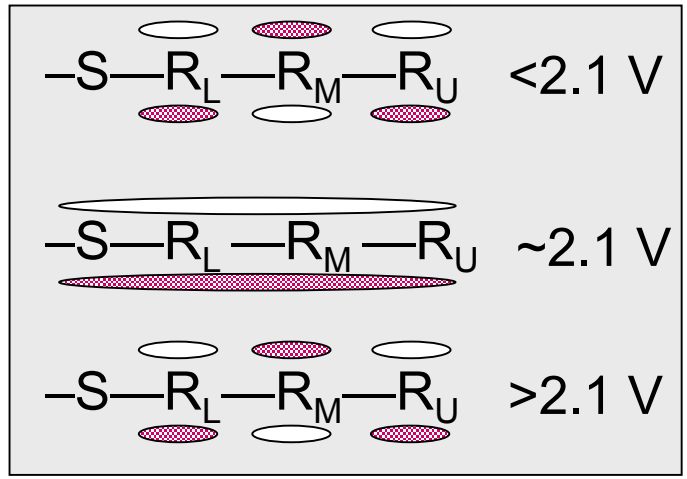
$$\{T+V_{hf}(r)+V_n(r) + V_x(r)\}\ \varphi_i = \varepsilon\ \varphi_i$$





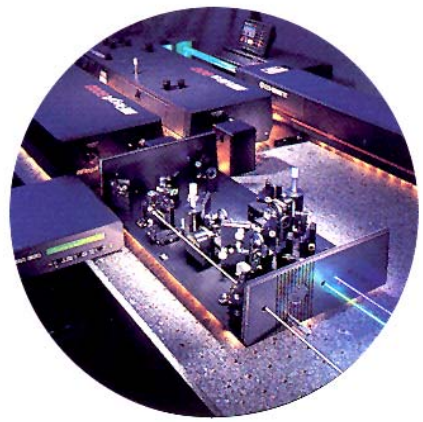
- Significant charge density localization at voltages below 2.1 V (no current).
- Near 2.1 V maximum de-localization of charge density (maximum current).
- Above 2.1 V charge density localization occurs again (no current).





The Road Ahead

- Small Ensemble Conduction Experiments
- Test Structure Assessment
- Electronic Structure Characterization
- Conduction Modeling

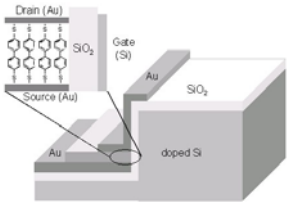


Leveraging our Resources

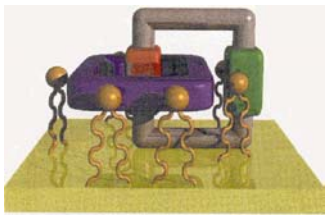
- **Nanocell Molecular Computer Collaboratory (Molecules, Electrical Characterization)**
  - –J. M. Tour, Rice University
  - –M.A. Reed, Yale University
  - –P.S. Weiss, Penn State University
- **Hewlett-Packard Research Labs (Devices, Electronic Structure)**
  - –R.S. Williams
  - –P.J. Kuekes
- **Naval 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