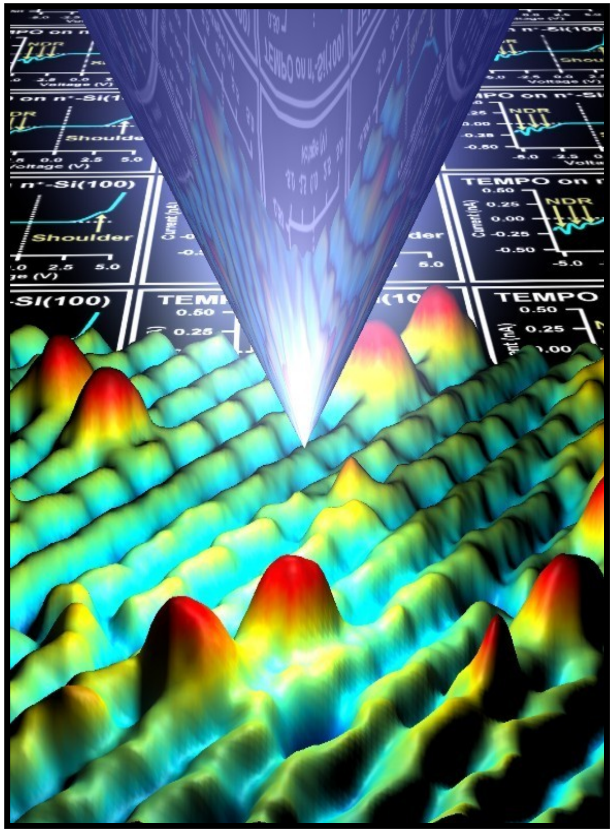
Electrical Contacts at the Nanometer Scale



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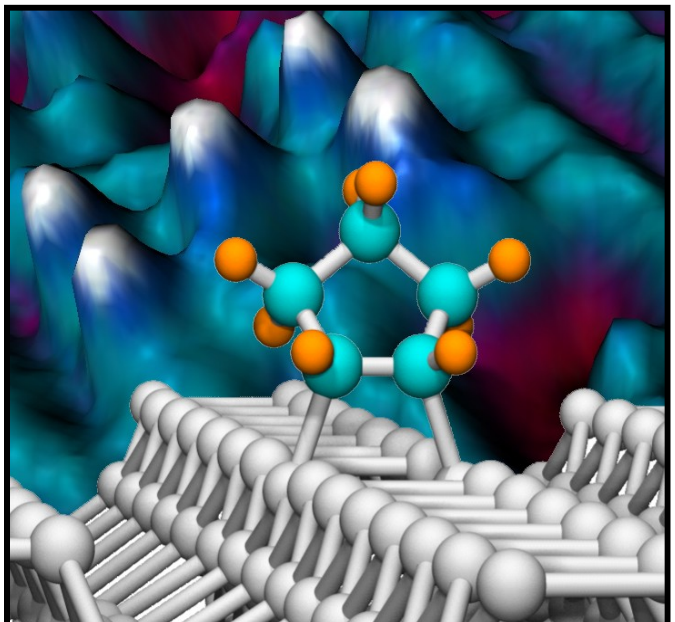
52nd IEEE Holm Conference

Montreal, Canada
September 27, 2006

Hersam Group Research Overview

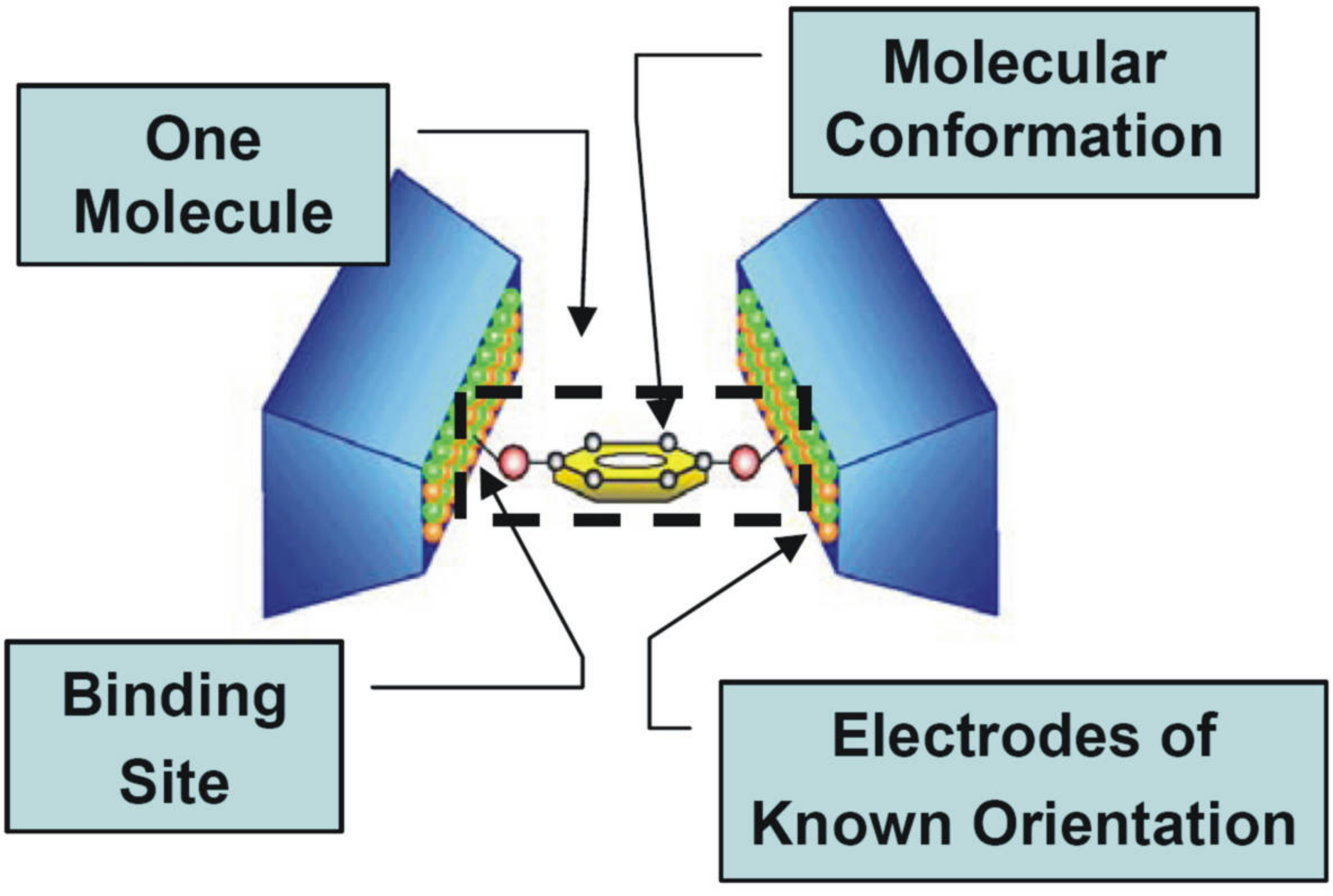
Overall goal: Explore the interface between materials science and chemistry down to the single molecule level



- Observe binding and conformation on surfaces
- Study electrical, mechanical, optical, and chemical properties
- Control surface reactivity with atomic precision

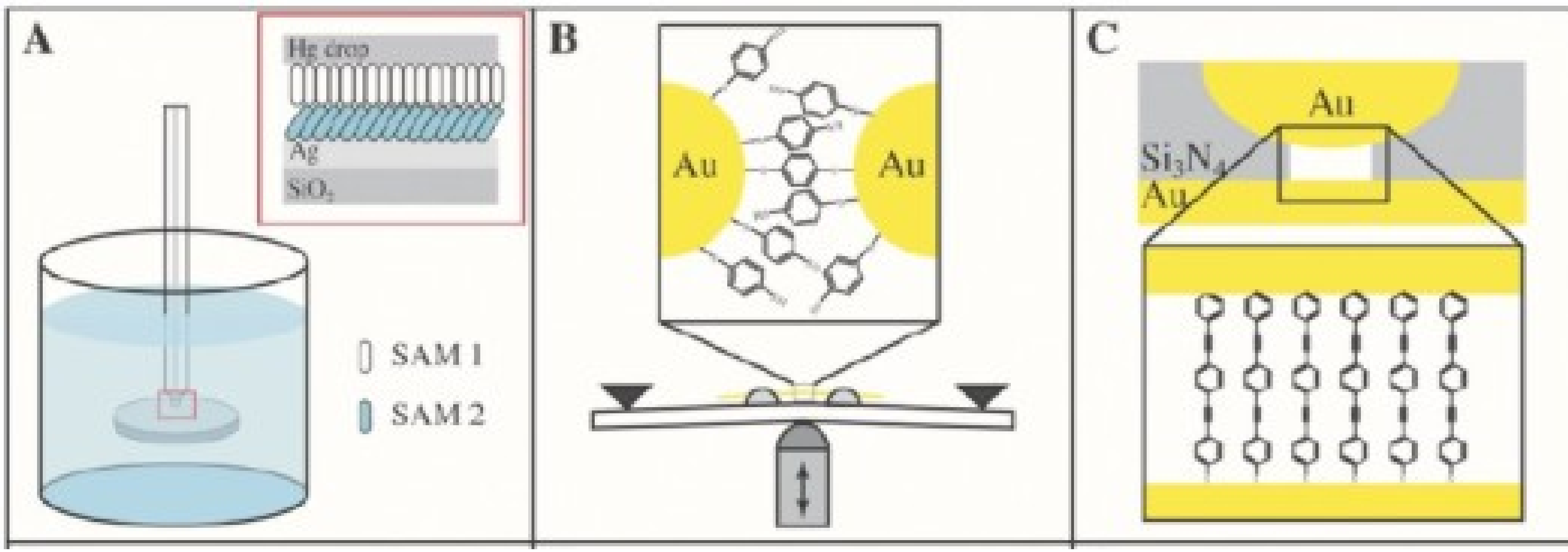
→ Structure → Properties → Processing ↩

An Ideal Experiment for Probing Molecular Conduction



M. C. Hersam, *et al.*, *MRS Bulletin*, **29**, 385 (2004).

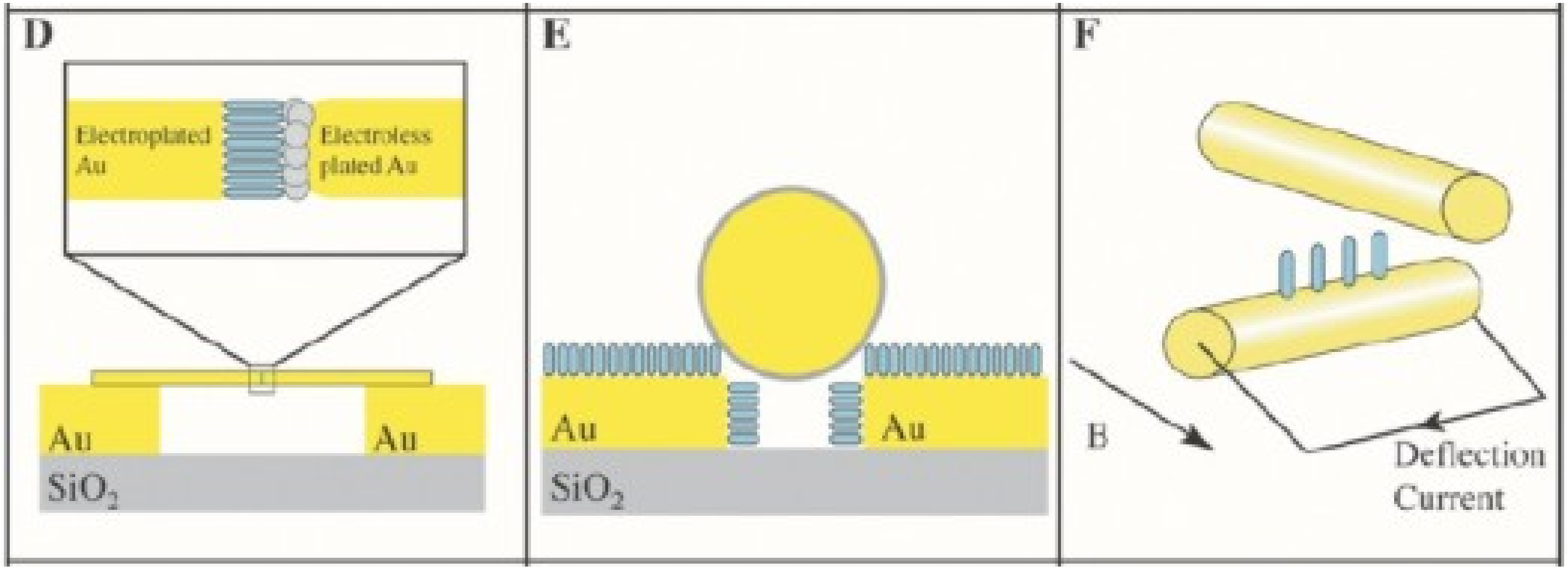
Real Experimental Strategies for Probing Molecular Conduction



Mercury Drop | **Mechanical Break Junction** | **Nanopore**

B. A. Mantooth, *et al.*, *Proc. IEEE*, **91**, 1785 (2003).

Real Experimental Strategies for Probing Molecular Conduction



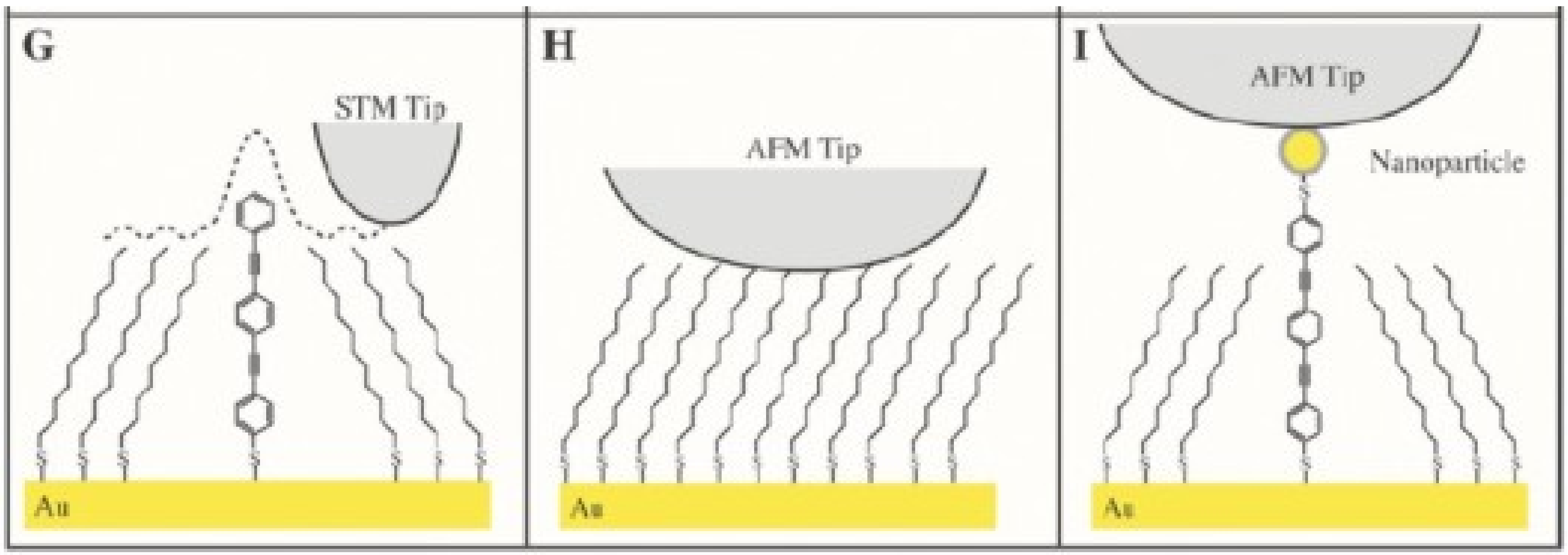
In-Nanowire Junction

Nanoparticle Junction

Crossed Nanowires

B. A. Mantooth, *et al.*, *Proc. IEEE*, **91**, 1785 (2003).

Real Experimental Strategies for Probing Molecular Conduction



Scanning Tunneling Microscopy

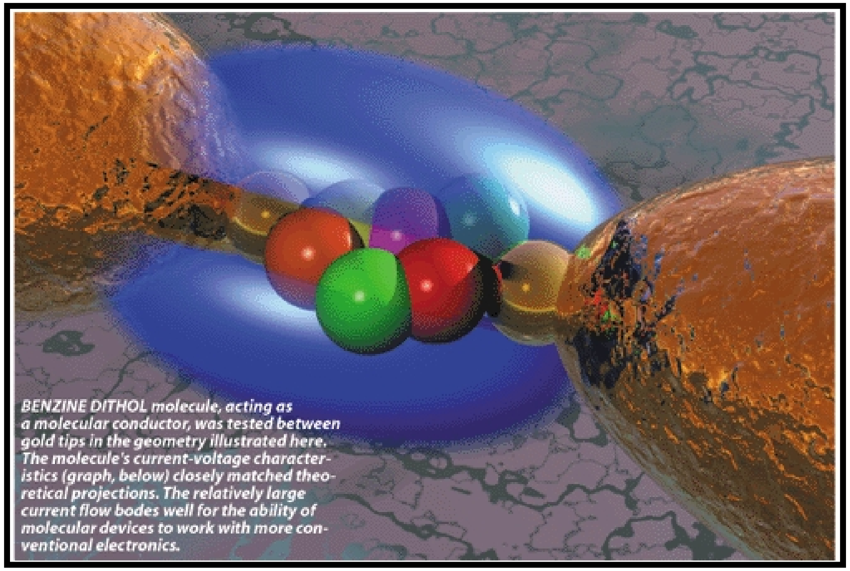
Conductive Atomic Force Microscopy

Conductive AFM + Nanoparticle

B. A. Mantooth, *et al.*, *Proc. IEEE*, **91**, 1785 (2003).

Recent Molecular Electronics Research

Metal-Molecule-Metal (Au-Thiol-Au) Junctions:



Sci. American, **282**, 86 (2000).

Recent results suggest that the contacts play a large – if not dominant role – in molecular electronic devices.

Science, **300**, 1384 (2003).

Alternative Approach: Molecules on Silicon

Objective: Study the effect of a semiconductor electrode on charge transport through single molecules.

Why Silicon?

- Established covalent organic binding chemistry
- Doping is easily controlled and well understood
- Band gap enables new charge transport mechanisms
- Technologically significant material for microelectronics

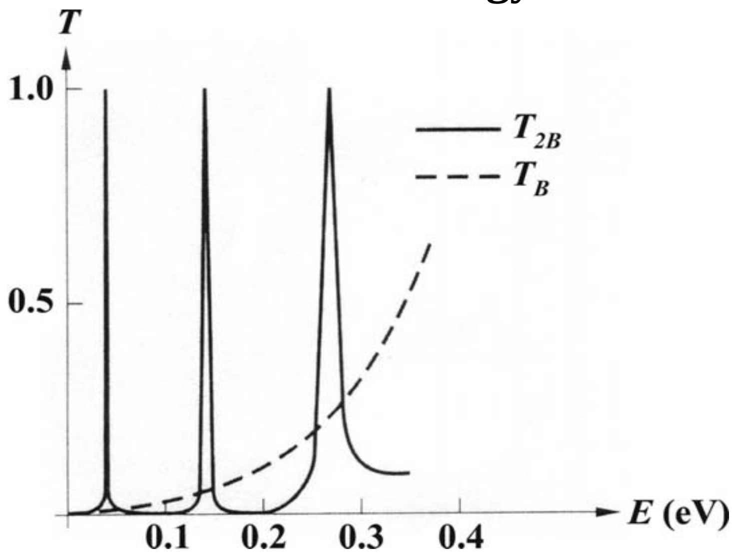
Proposed Device: Molecular RTD

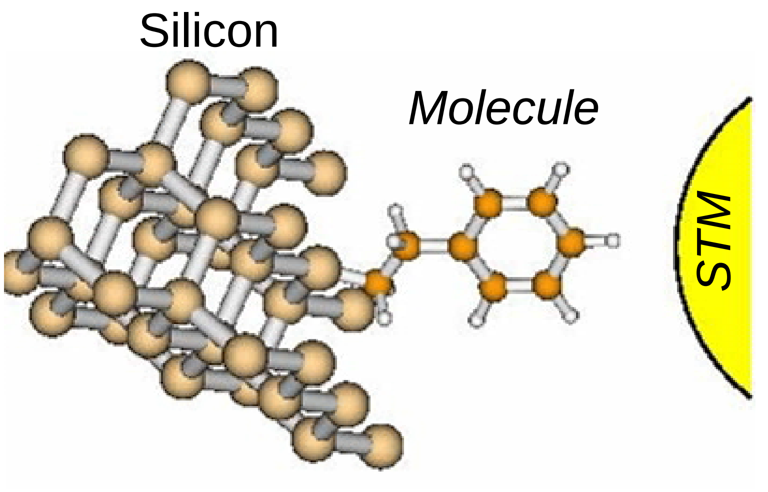
Collaboration with Supriyo Datta: *Nano Letters*, **4**, 1803 (2004).

Molecular Resonant Tunneling Diode (RTD):

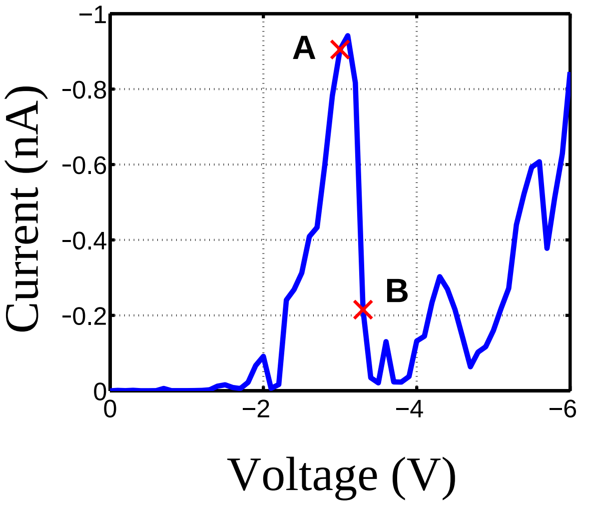
Negative Differential Resistance (NDR)

Tunneling probability versus energy:

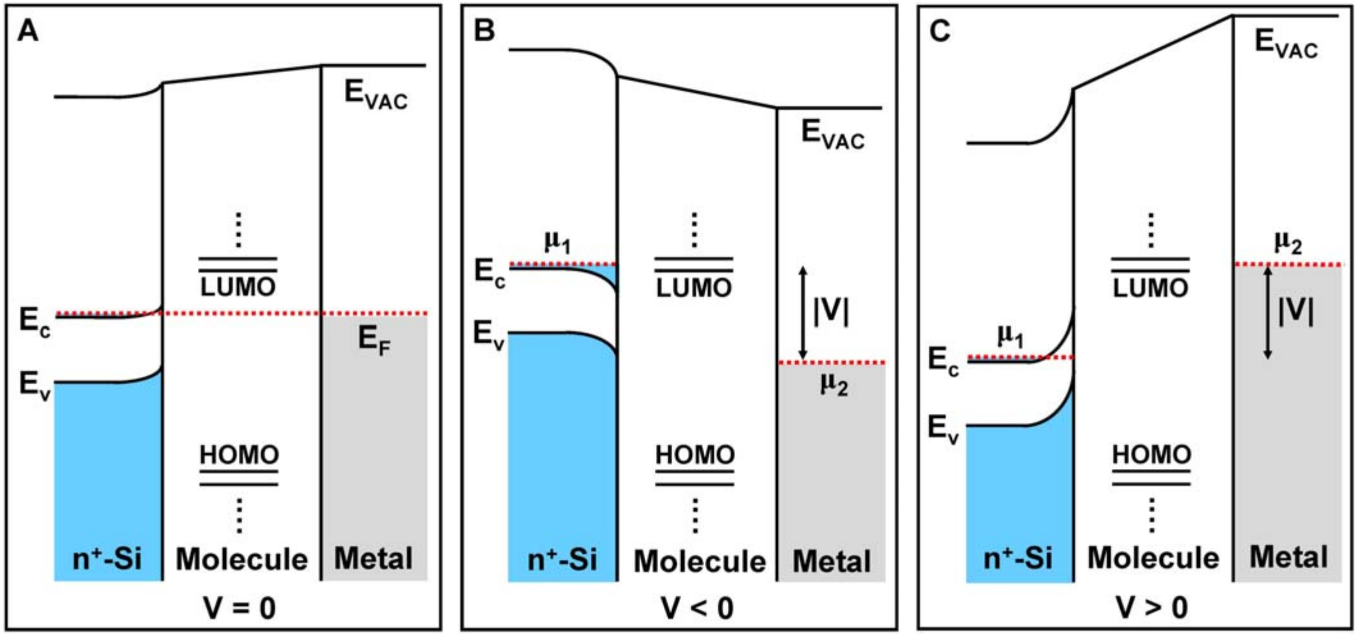




Calculated I-V Curve:



Band Diagrams for Molecules on n+-Si



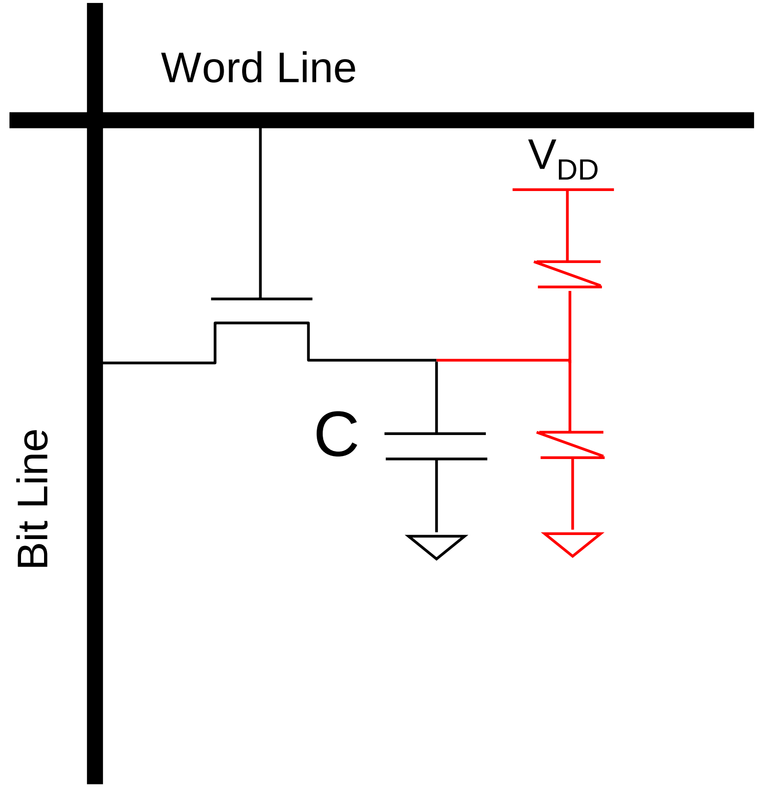
Equilibrium **NDR** **Shoulder**

The presence of the semiconductor band gap enables negative differential resistance in this model.

Potential Applications of RTDs

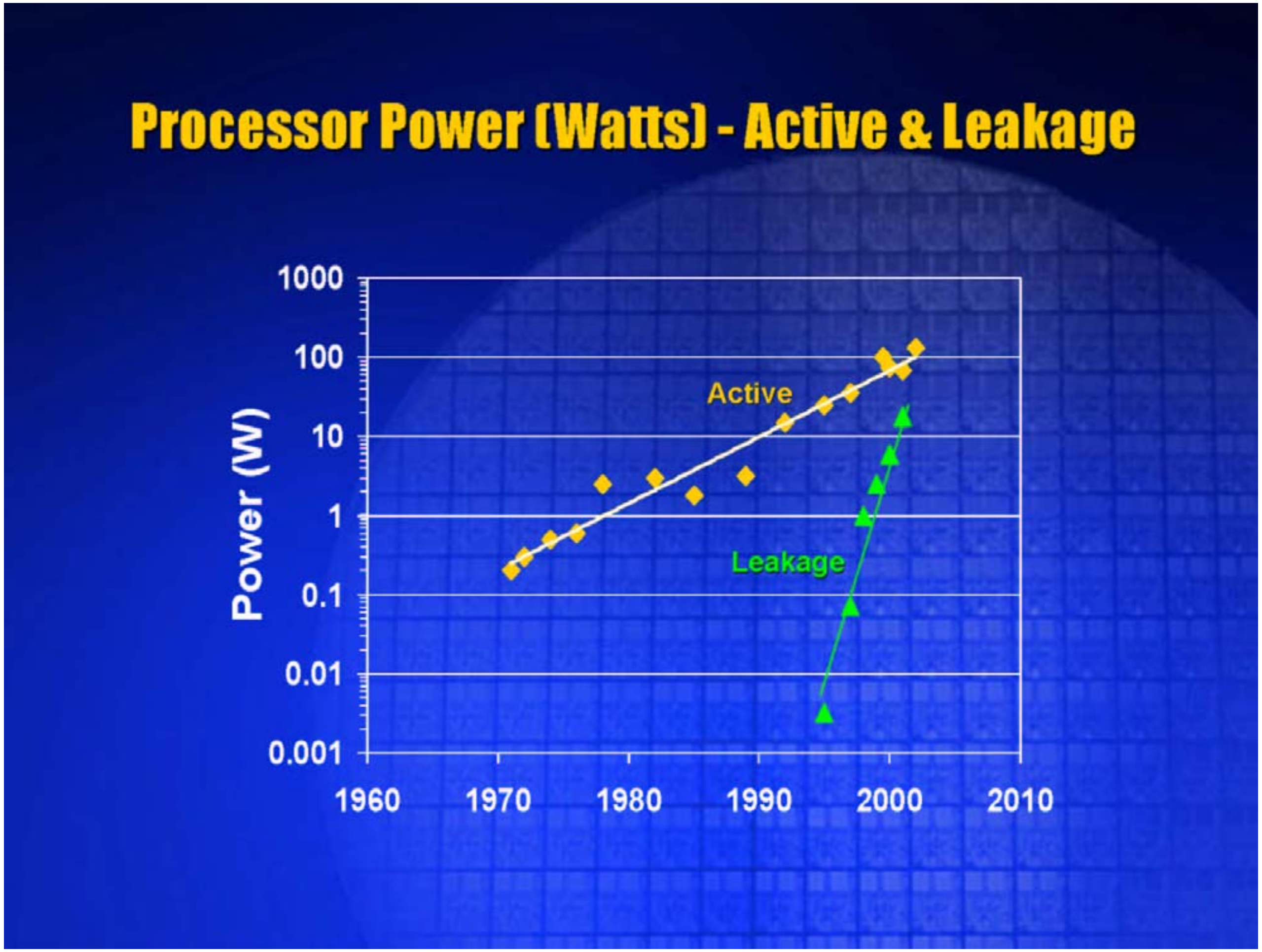
- RTD-FET logic
  Seabaugh, et al., 1997
  Mathews et al., 1999

- RTD refresh for DRAMs
  Seabaugh, et al., 1998
  Berg et al., 2000



Combining resonant tunneling diodes with conventional silicon transistors enables computing with reduced power dissipation.

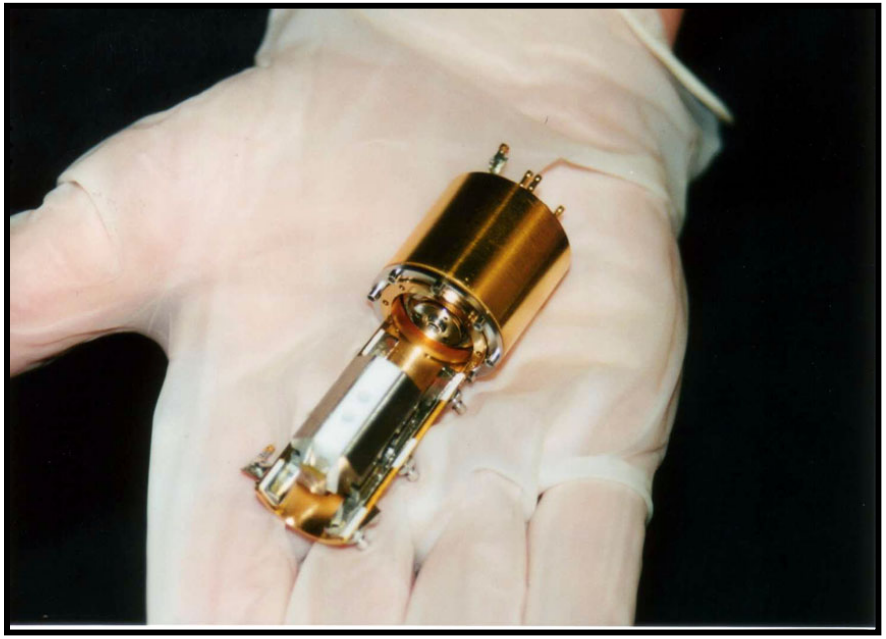
Moore's Law for Power Consumption

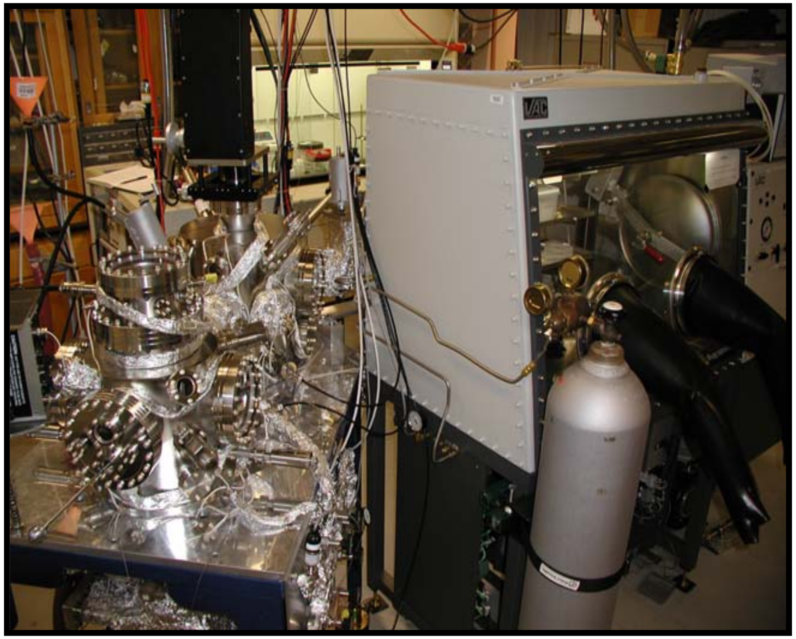


"No Exponential is Forever … but We Can Delay 'Forever',"
Gordon E. Moore, International Solid State Circuits Conference, Feb. 10, 2003.

UHV STM Measurements

Review of Scientific Instruments, **75**, 5280 (2004).

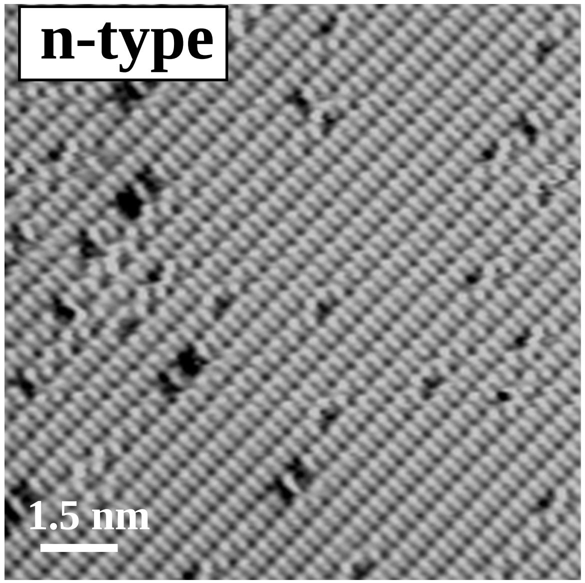


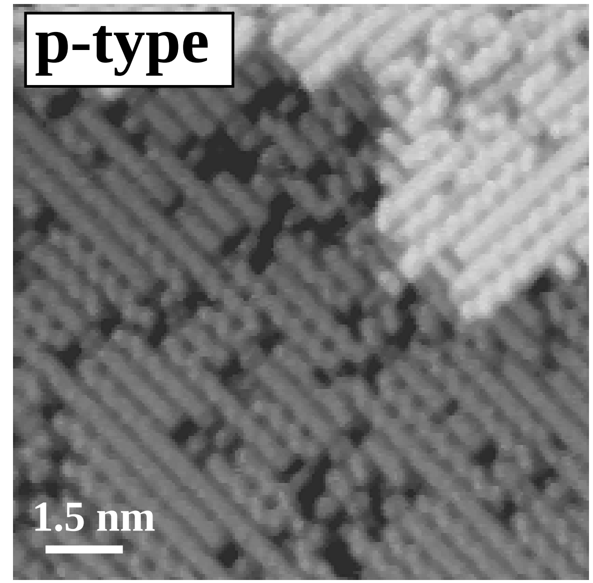


- Fundamental scanning tunneling microscopy experiments in ultra-high vacuum at room temperature
- Homebuilt UHV STM directly interfaced to a controlled atmosphere glove box

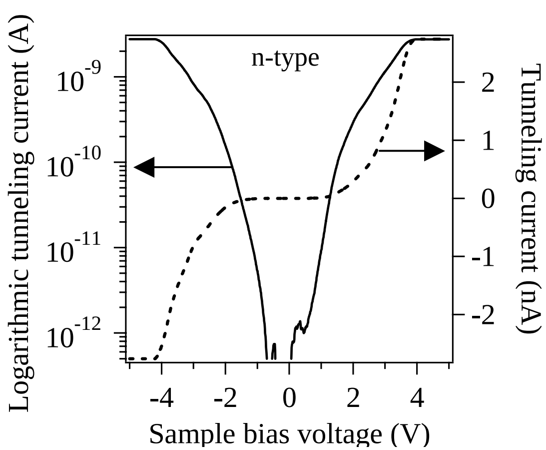
Degenerately Doped Si(100)-2×1 Surfaces

Nanotechology, **15**, S452 (2004).

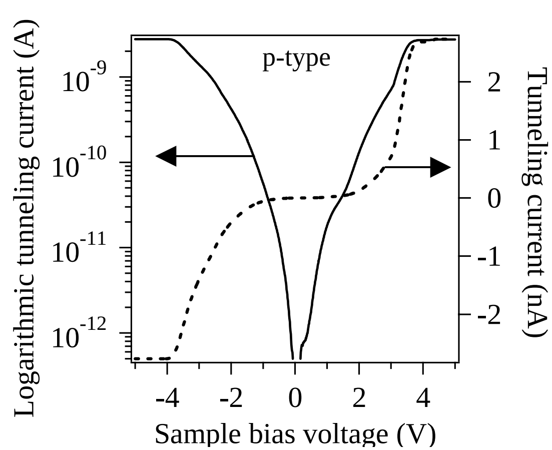




(c)



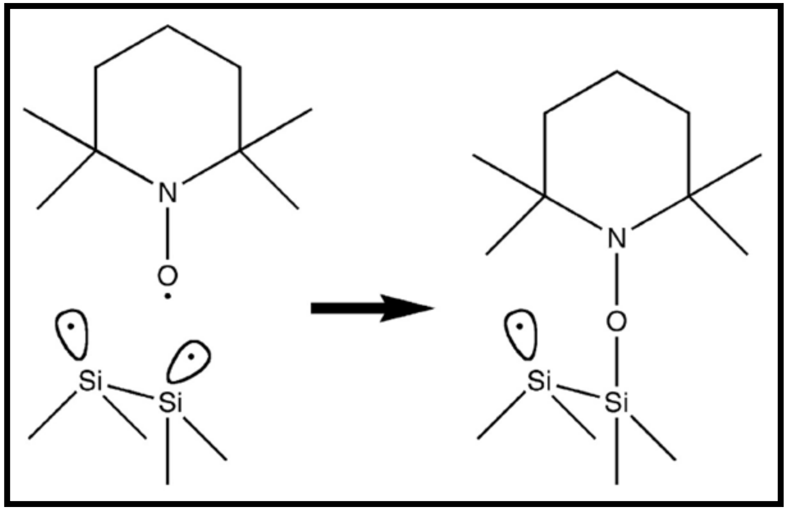
(d)



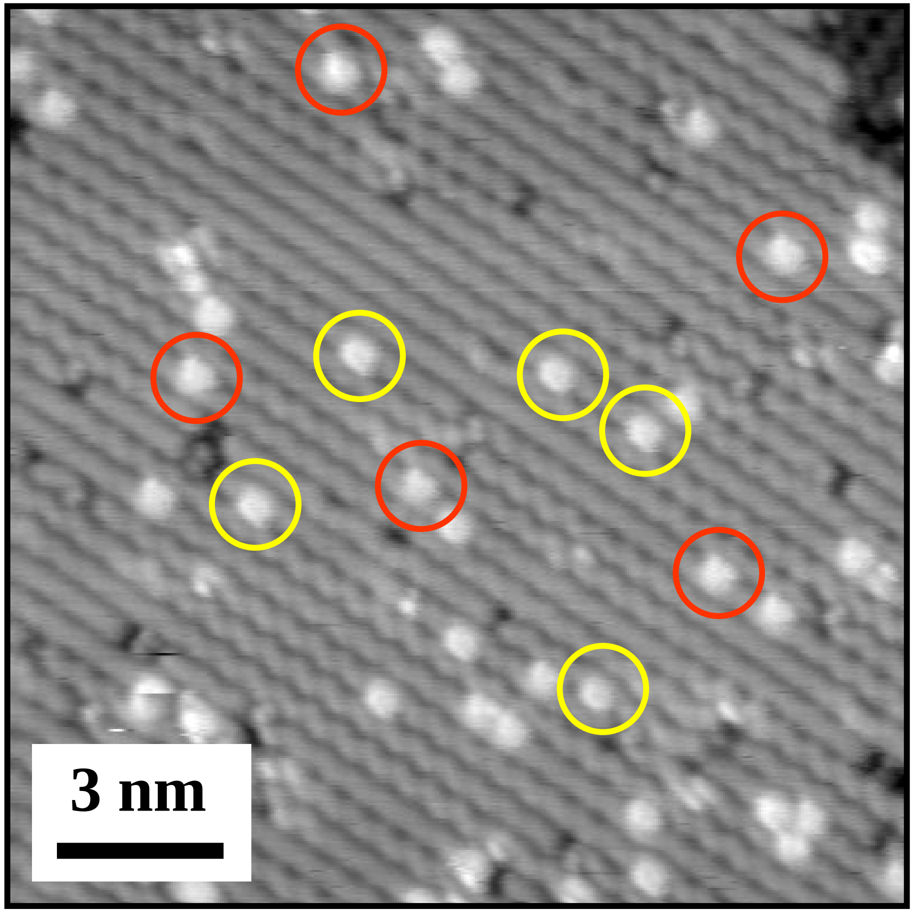
TEMPO Adsorption on Si(100)

Surface Science, **559**, 16 (2004).

TEMPO - (2,2,6,6-tetramethyl-1-piperidinyloxy)



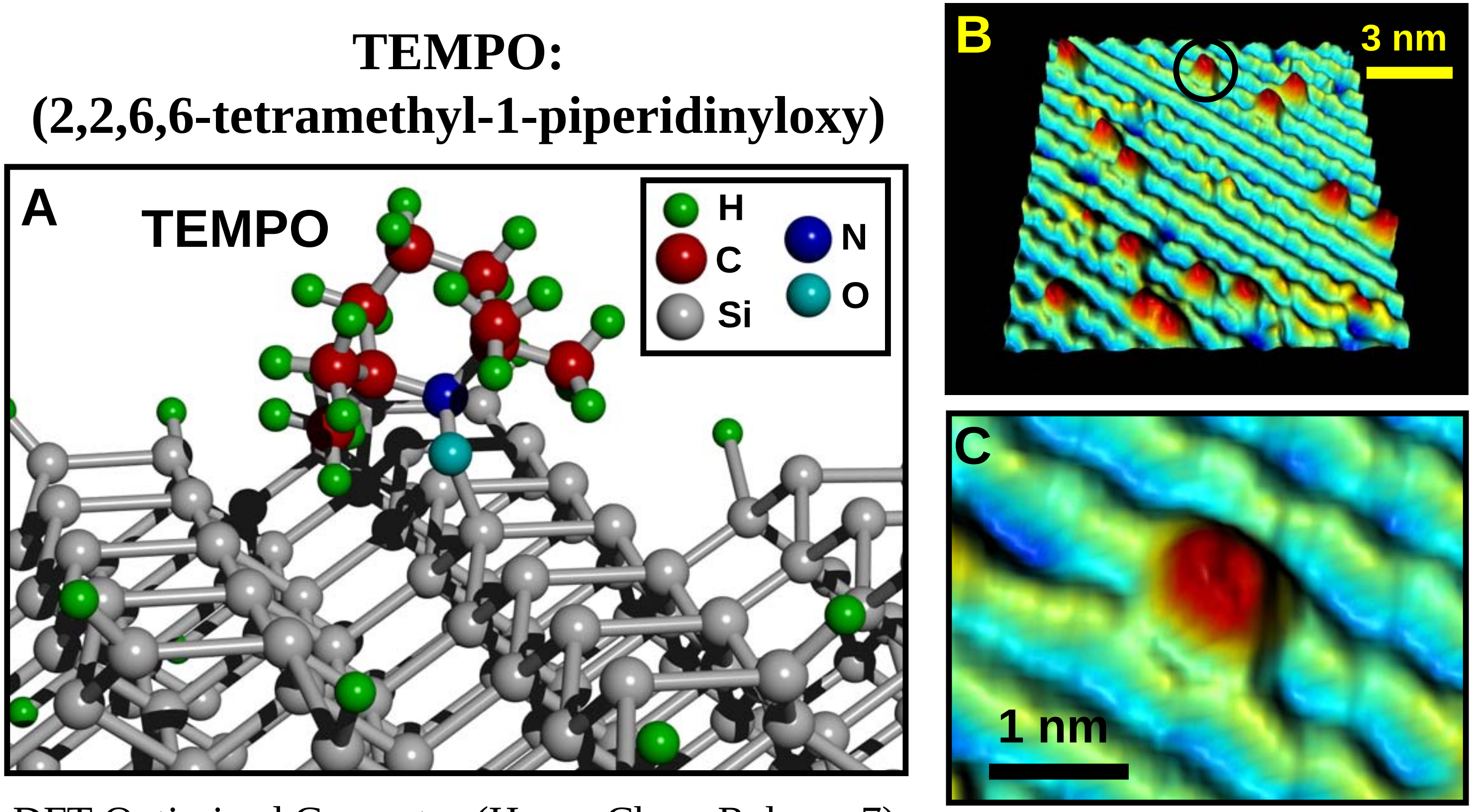
The nitroxyl free radical reacts with only one dangling bond on the silicon dimer.



TEMPO on the Si(100)-2×1 Surface

Nano Letters, **4**, 55 (2004).

TEMPO:
(2,2,6,6-tetramethyl-1-piperidinyloxy)

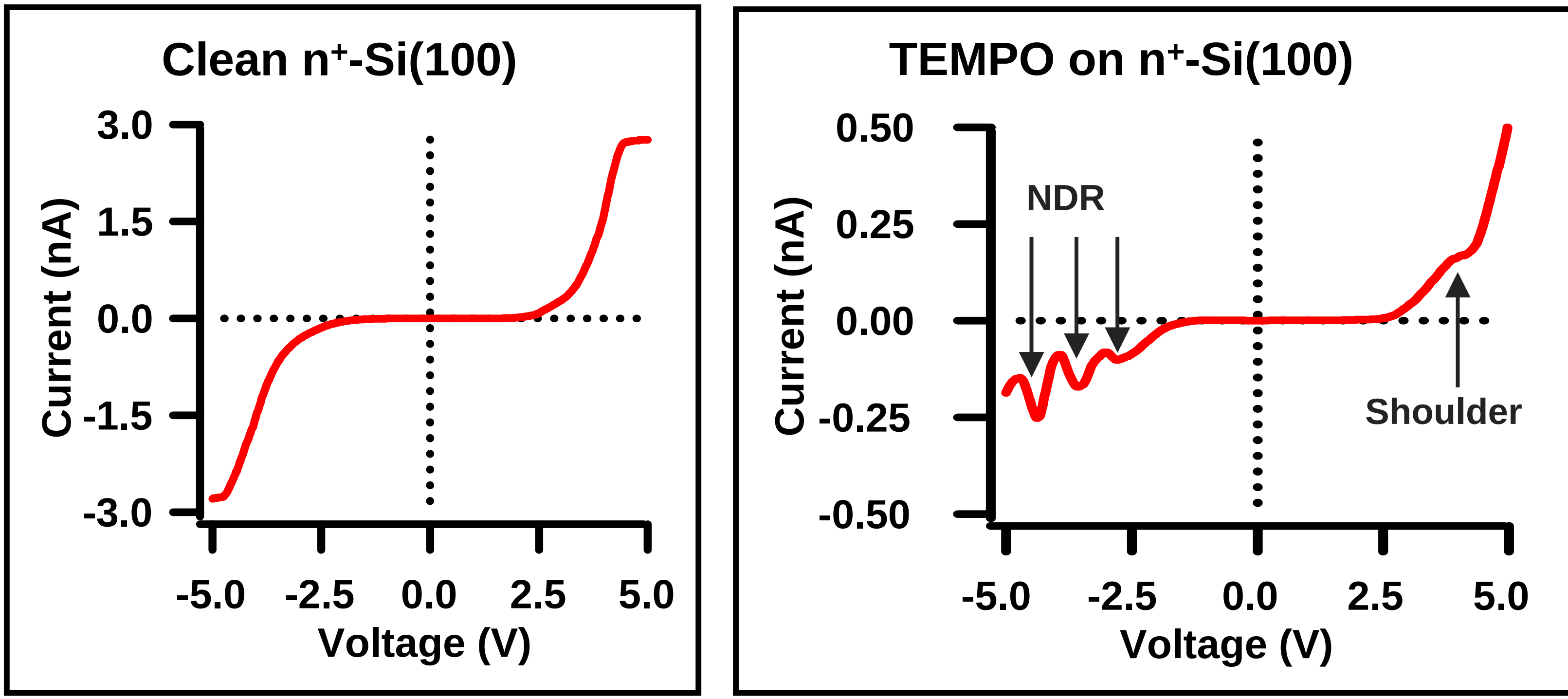


DFT Optimized Geometry (Hyper Chem Release 7)

Individual TEMPO molecules are probed with the STM

I-V Curve for TEMPO on n+-Si(100)

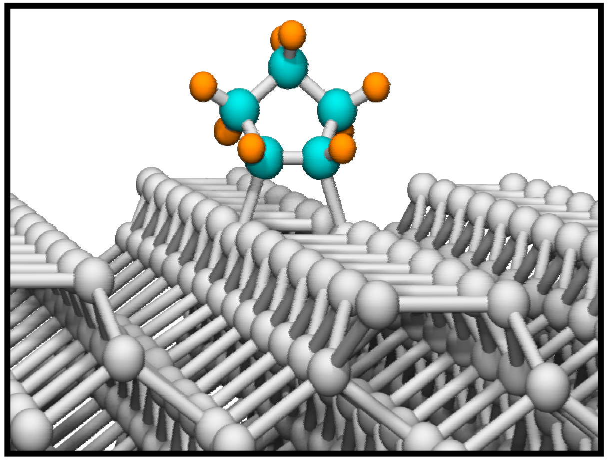
Nano Letters, **4**, 55 (2004).

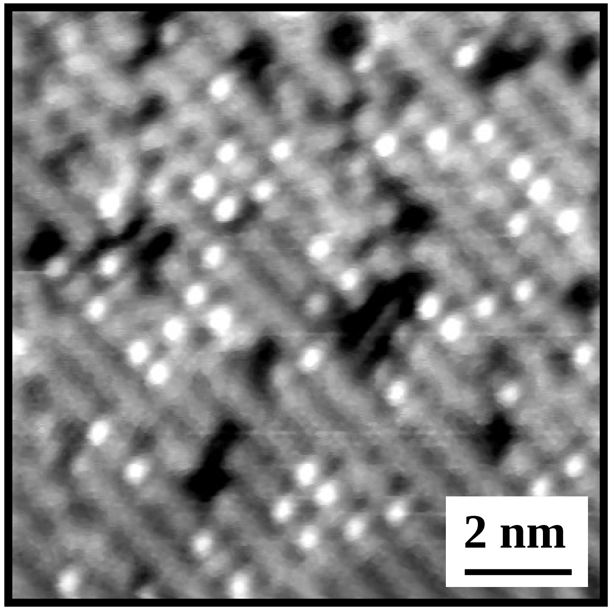


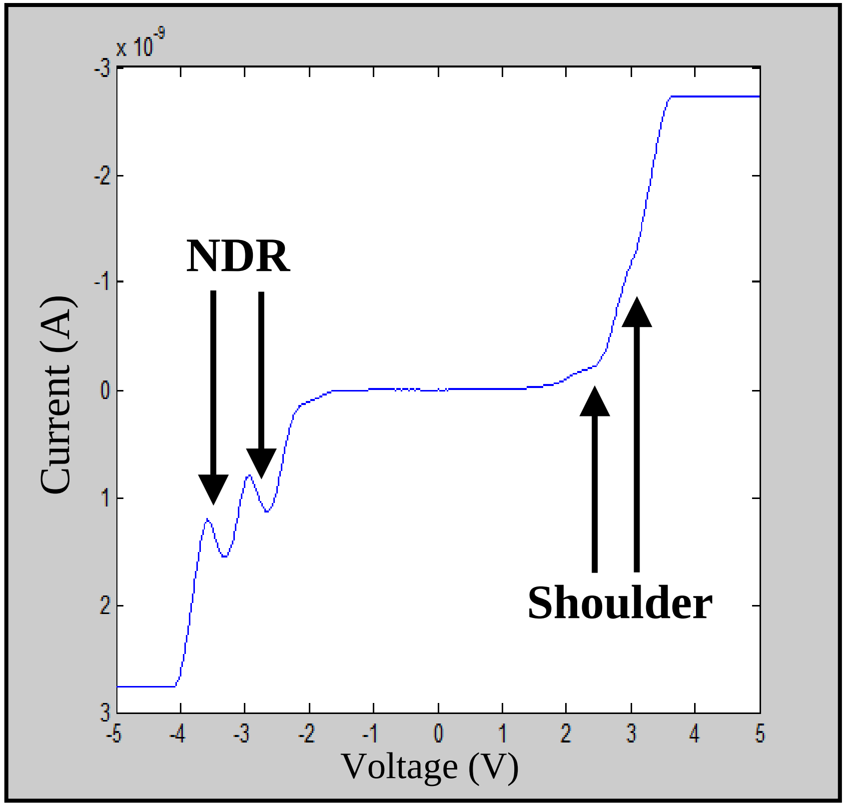
- NDR events are only observed at negative sample bias.
- Shoulder is only observed at positive sample bias.

Cyclopentene on n$^+$-Si(100)

Nanotechnology, **15**, S452 (2004).

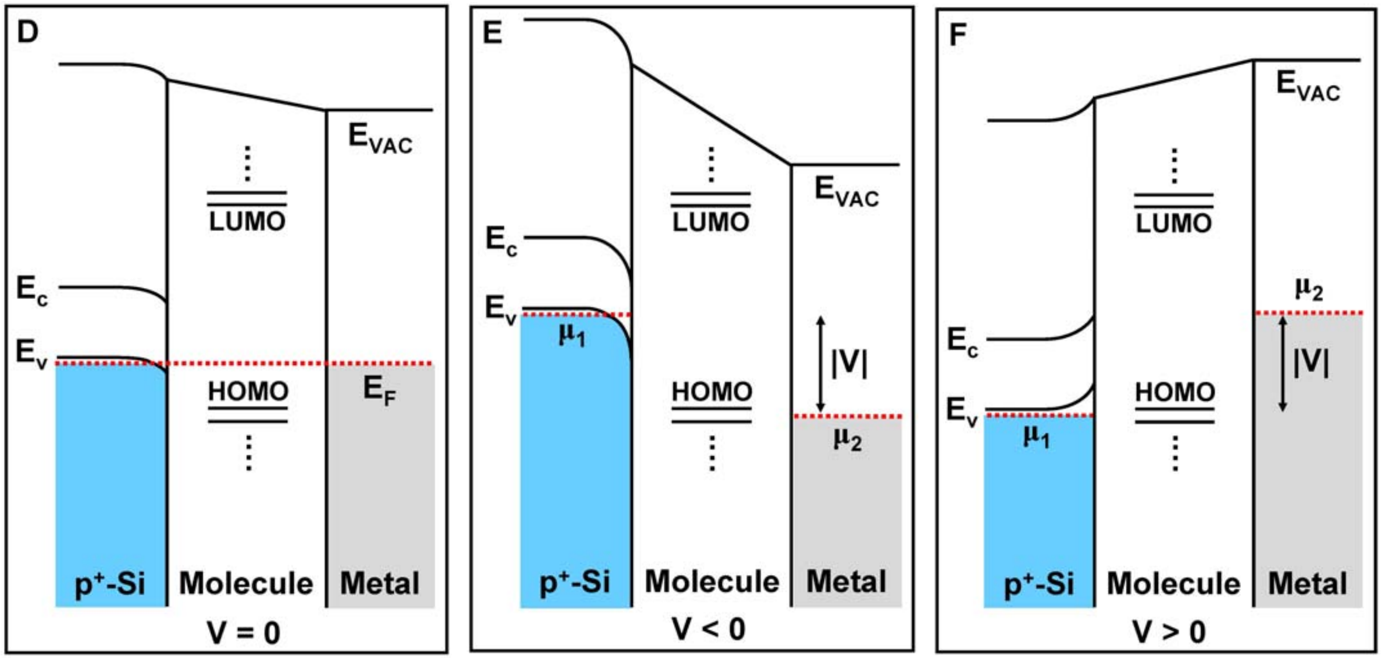






NDR observed on an isolated cyclopentene molecule on n$^+$-Si(100)

Band Diagrams for Molecules on p+-Si

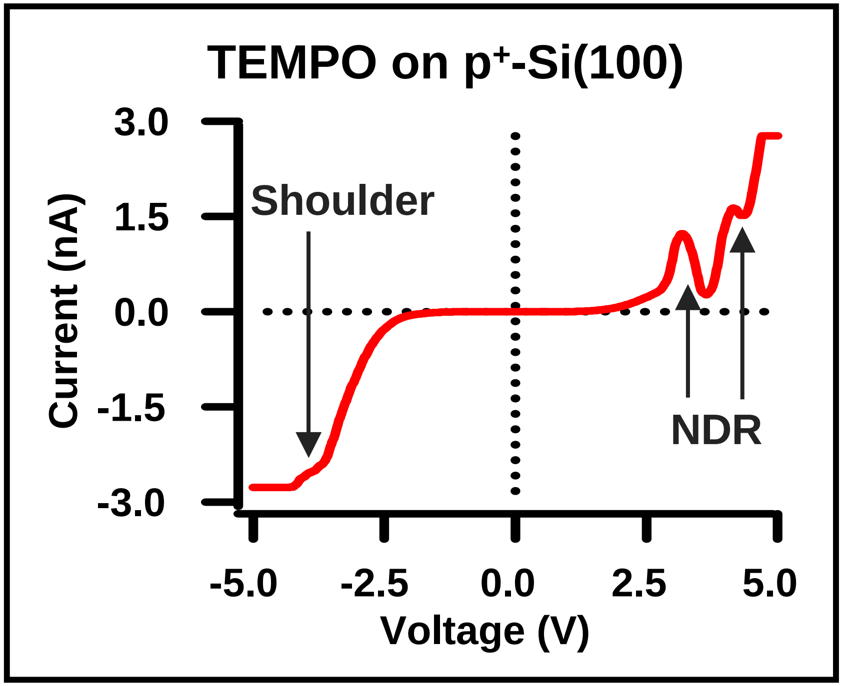


Equilibrium **Shoulder** **NDR**

Qualitatively similar behavior as n^+-Si except at the opposite bias polarity.

I-V Curve for TEMPO on p⁺-Si(100)

Nano Letters, **4**, 55 (2004).

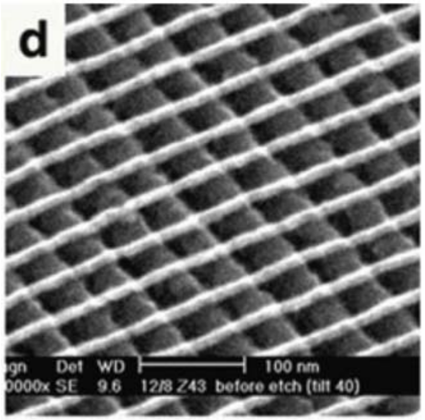


- Qualitative agreement with band diagrams.
- Quantitative agreement with theory requires answers to the following questions:

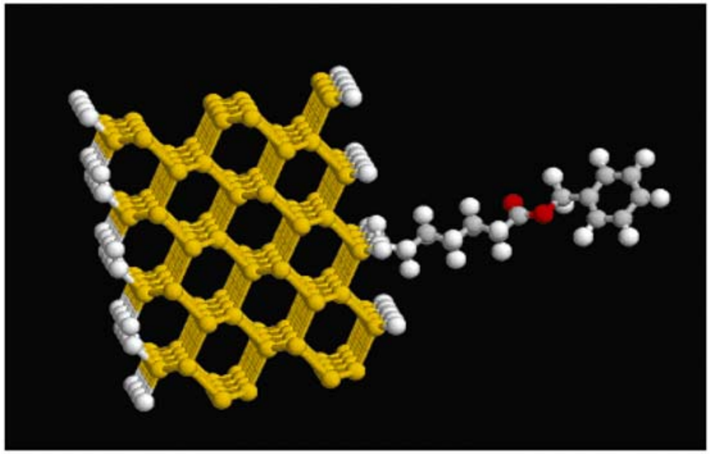
What are the energies of the molecular orbital levels with respect to the semiconductor bandstructure?

How does the voltage drop across the semiconductor-molecule-vacuum-metal junction?

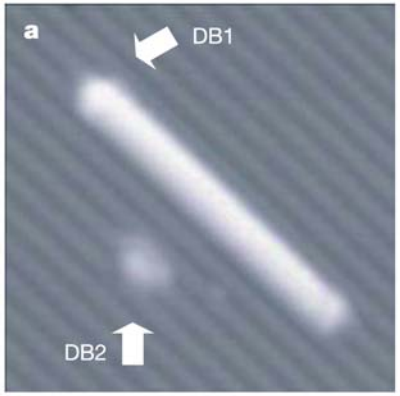
Recent Silicon-Based Molecular Electronics Research



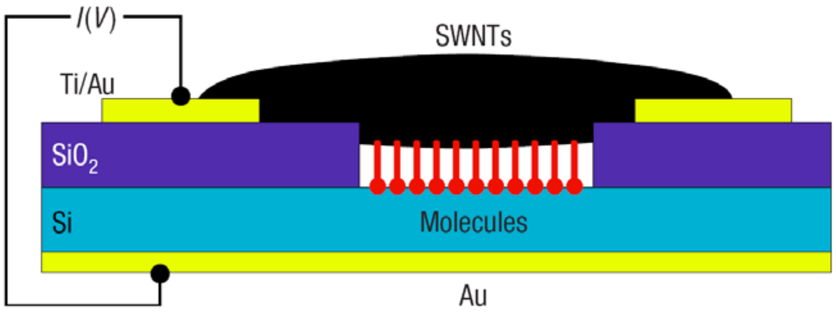
Rotaxanes on poly-Si
Stoddart and Heath, Faraday Discuss., 2006



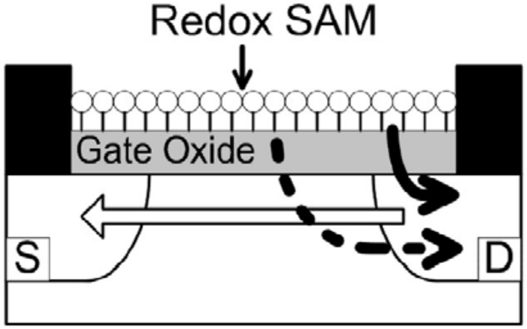
Si-based molecular rectifying diode
Vuillaume, Nano Lett., 2003



Styrene chains on Si
Wolkow, Nature, 2005



Si-molecule-nanotube testbed
Tour, Nature Materials, 2005



Redox SAM memory on Si
Misra, IEEE Nano, 2006

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