

Nano-Electronics and Bio-Electronics

Deepak Srivastava
 NASA Ames Research Center
 MS T27A-1 and MS 229-3
 Moffett Field, CA 94034-1000

deepak@nas.nasa.gov, (650) 604-3486

<http://www.ipt.arc.nasa.gov>
<http://www.nas.nasa.gov/~deepak/home.html>

Why Nanotechnology at NASA?

- Advanced miniaturization, a key thrust area to enable new science and exploration missions
 - Ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed
- Revolutions in electronics and computing will allow reconfigurable, autonomous, "thinking" spacecraft
- Nanotechnology presents a whole new spectrum of opportunities to build device components and systems for entirely new space architectures
 - Networks of ultrasmall probes on planetary surfaces
 - Micro-rovers that drive, hop, fly, and burrow
 - Collection of microspacecraft making a variety of measurements

NASA Ames Nanotechnology Program

- Started in FY 97, currently about 25 FTEs on site working on nanotechnology research: additional 15 FTEs involved in simulation, process modeling, and computational chemistry
- Research focus ranges from carbon and protein nanotubes, quantum device physics, quantum computing, data storage to optoelectronics, DNA electronics, Bio-Sensors, Bacteriorhodopsin-based Data-Storage
- Largest carbon nanotube effort in the Federal government and also one of the largest in the world
 - About ~60 refereed publications in the field
 - Over 100 talks in National/International Meetings
 - Two Feynmann Awards

Research Focus

Nanotechnology Nanotubes - Controlled, patterned growth of CNT - Large scale production of CNT - Hydrogen storage in nanotubes - CNT-based biosensor for cancer diagnostics - Functionalization of nanotubes - AFM study of Mars dust - AFM study of Mars meteorite - CNT-based sensor for astrobiology - Protein nanotubes: growth and applications - Reactor/Process Modeling of CNT growth - Computational investigation of electronic, mechanical and other properties of CNT - Transport in CNT, Nanoelectronics - BN nanotubes, structure and properties - Design of CNT-based mechanical components	- Chemical Storage of Data - Atomic Chain Electronics - Bacteriorhodopsin based holographic data storage Computational Electronics, Computational Optoelectronics - Development of multidimensional quantum simulators to design ultrasmall semiconductor devices - Development of semiclassical methods with quantum correction terms - Investigation of device technologies suitable for petaflop computers - Modeling of optoelectronics devices, VCSEL, THz modulation - Optical interconnect modeling
---	--

What is Expected from Alternative Electronic Technologies?

- Must be easier and cheaper to manufacture than CMOS
- Need high current drive: should be able to drive capacitances of interconnects of any length
- High level of integration (10^9 transistors/circuit)
- High reproducibility (better than $\pm 5\%$)
- Reliability (operating time > 10 years)
- Very low cost (< 1 μ cent/transistor)
- Everything about the new technology must be compelling and simultaneously CMOS scaling should fail. If these two together do not happen, the enormous infrastructure built around silicon will make it difficult for alternatives to emerge.

Carbon Nanotube

CNT is a tubular form of carbon with diameter as small as 1 nm. Length: few nm to microns.

CNT is configurationally equivalent to a two dimensional graphene sheet rolled into a tube.

CNT exhibits extraordinary mechanical properties: Young's modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.

CNT can be metallic or semiconducting, depending on chirality.




Potential CNT Applications and Challenges

Source: Workshop Report - SRC/NASA Ames Workshop on Emerging Opportunities and Issues in Nanotubes and Nanoelectronics

Application	Property	Challenge
CNT for active electronic devices	Feasibility to control electronic properties by structural characteristics	The current standards should be met, low cost (10^6 molecules/cm ²), high reproducibility (10^6 molecules/cm ²), high reproducibility (10^6 molecules/cm ²), high reproducibility (10^6 molecules/cm ²)
CNT as interconnects	Low resistivity	Is it possible to grow helical conducting nano tubes?
Passive devices, capacitors and inductors	Geometrical characteristics	Performance of CNT field effect transistors
Field emitters	High aspect ratio, thermal conductivity	The CNT film would need to be deposited, patterned, patterned and etched with techniques compatible with the underlying silicon devices
CNT film as a low-E insulator	achieve low density of the CNT film	Attachment of a single CNT to the substrate
Probes for microscopy	High aspect ratio of tips	Micro-and arrays must be "fast, flexible, and inexpensive"
Manufacturing with Micro- or Nano-Tools	High aspect ratio of tips	

CNT Synthesis

- CNT has been grown by laser ablation (pioneering at Rice) and carbon arc process (NEC, Japan) - early 90s
 - SWNT, high purity, purification methods
- CVD is ideal for patterned growth (electronics, sensor applications)
 - Well known technique from microelectronics
 - Hydrocarbon feedstock
 - Growth needs catalyst (transition metal)
 - Multiwall tubes at 500-800° deg. C.
 - Numerous parameters influence CNT growth



Carbon Nanotubes at Ames





CNT in Microscopy

Atomic Force Microscopy is a powerful technique for imaging, nanomanipulation, as platform for sensor work, nanolithography...

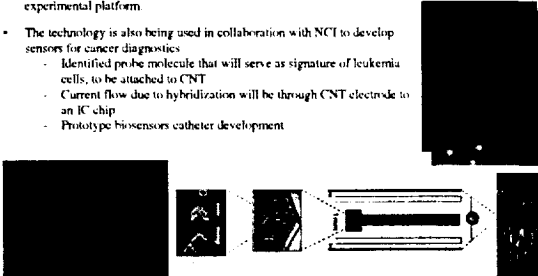
Conventional silicon or tungsten tips wear out quickly. CNT tip is robust, offers amazing resolution.





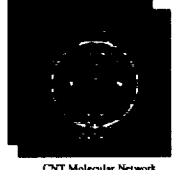
CNT Based Biosensors

- Our interest is to develop sensors for astrobiology to study origins of life. CNT, though inert, can be functionalized at the tip with a probe molecule. Current study uses AFM as an experimental platform.
- The technology is also being used in collaboration with NCI to develop sensors for cancer diagnostics
 - Identified probe molecule that will serve as signature of leukemia cells, to be attached to CNT
 - Current flow due to hybridization will be through CNT electrode to an IC chip
 - Prototype biosensors catheter development



Computational Nanotechnology

- Large scale computer simulations based on ab initio methods enable understanding nanotube characteristics and serve as design tool
 - Evaluation of mechanical properties
 - Evaluation of electronic properties
 - Electron transport in CNT devices
 - Functionalization of the nanotubes
 - Design of electrical and mechanical devices
 - Evaluation of storage potential (H₂, Li)





www.nas.nasa.gov/~deepak/home.html



Ames Research Center

Computational Nanotechnology



2- point Nanotube Heterojunctions

Molecular Electronic Switches




(0,0) - (0,0)

(0,0) - (0,0)

(0,0) - (0,0)

(0,0) - (0,0)

Bent Junctions **Straight Junctions**

*Chen et al. Phys. Rev. Lett. 86
Chen et al. J. Phys. Chem. B 96
Lundberg et al. J. Chem. Phys. 106
Saba et al. Phys. Rev. B 56*

Pathways to Two Dimensional Molecular "Nanowires"




Y-Junctions **Central Defect**

*Chen et al. Phys. Rev. Lett. 86
Chen et al. J. Phys. Chem. B 96
Lundberg et al. J. Chem. Phys. 106
Saba et al. Phys. Rev. B 56*

We studied the effect of coupling the tubes and relaxing the junctions with a quantum DFT-MD method.

"It turns out that all of our proposed junctions actually do conduct."
John's **Lab** shows the **gold** **working** of **computer** **models** **of** **nanowires**.

Ames Research Center

Computational Nanotechnology

Wire and clips

Nanotechnology Device

"Nanotechnology is the world's future."

- Assembly is self-assembly through shape and relax interactions
- Provision for molecular interconnection to the outside molecular circuitry

Atomic Chain Electronics

Smallest electronics with precise structures

Monolayer $\sim 10^6$ Å

Uniform
Predictable
Controllable

Monolayer $\sim 10^6$ Å

Nonuniform
Unpredictable
Uncontrollable

Monolayer $\sim 10^6$ Å

Uniform
Predictable, accurate
Designable

Precise structures

Produced on a template

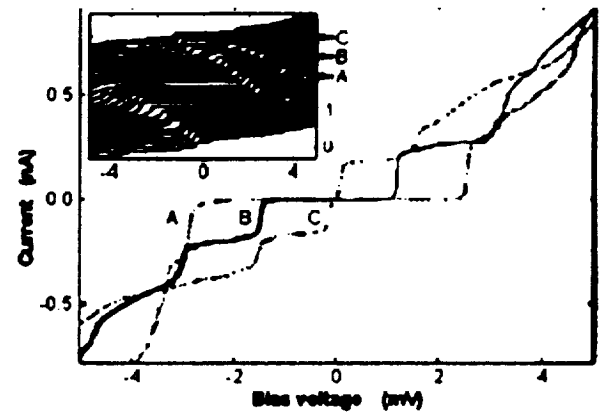
Monolayer
Monolayer

Fluencing at chemical bonding

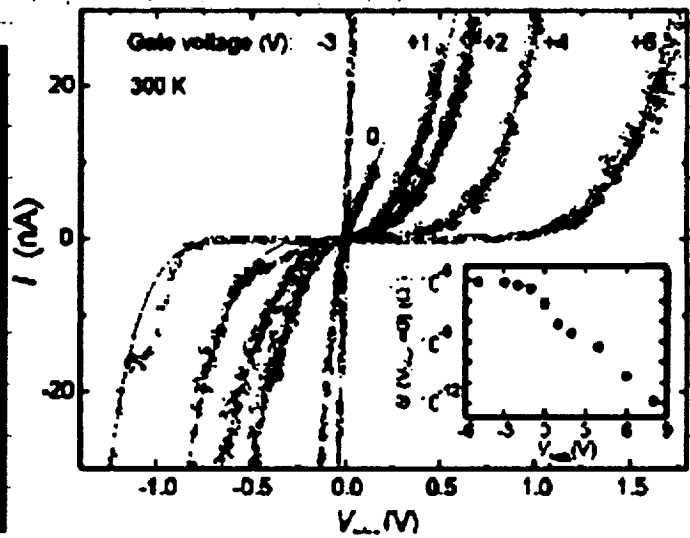
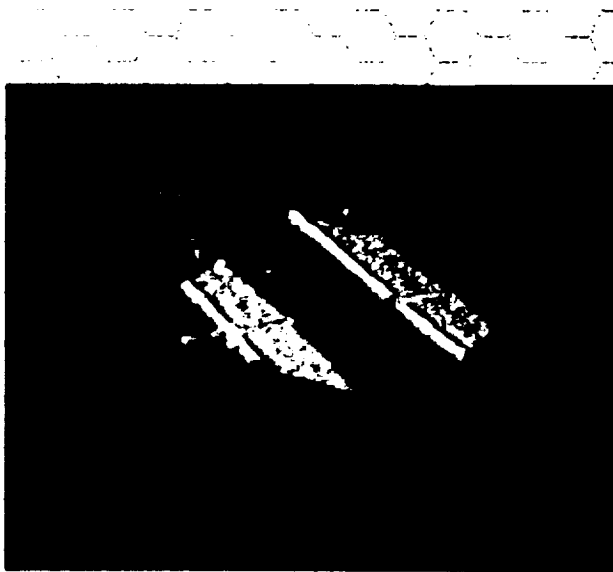
Tuning of controlled electronic properties

T.YAM, MDA

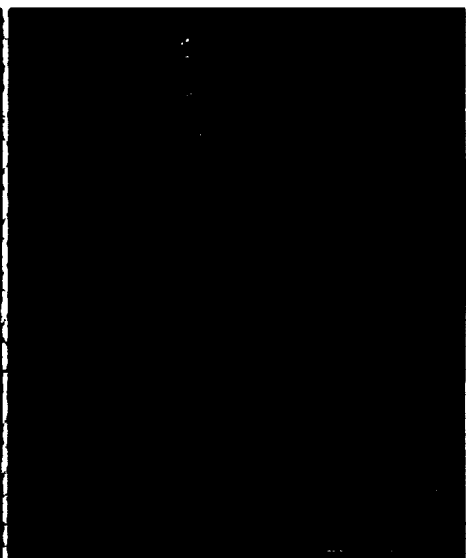
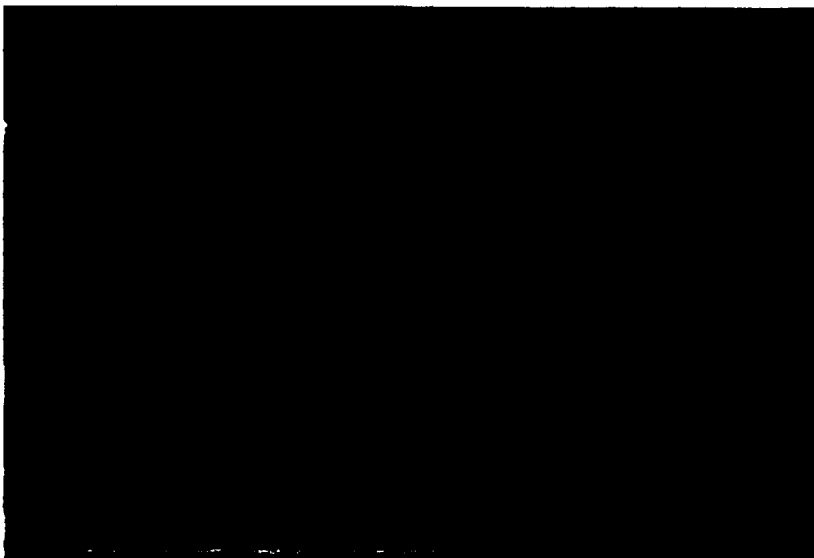
T.YAM, MDA



Nanotube as Quantum Molecular Wire (**Nature 1997**)



Nanotube Field Effect Transistor (**Nature 1998**)



Nanotube Hetero-Junctions (**Nature 1999**)

Electronic Transport in Y-Junction Carbon Nanotubes

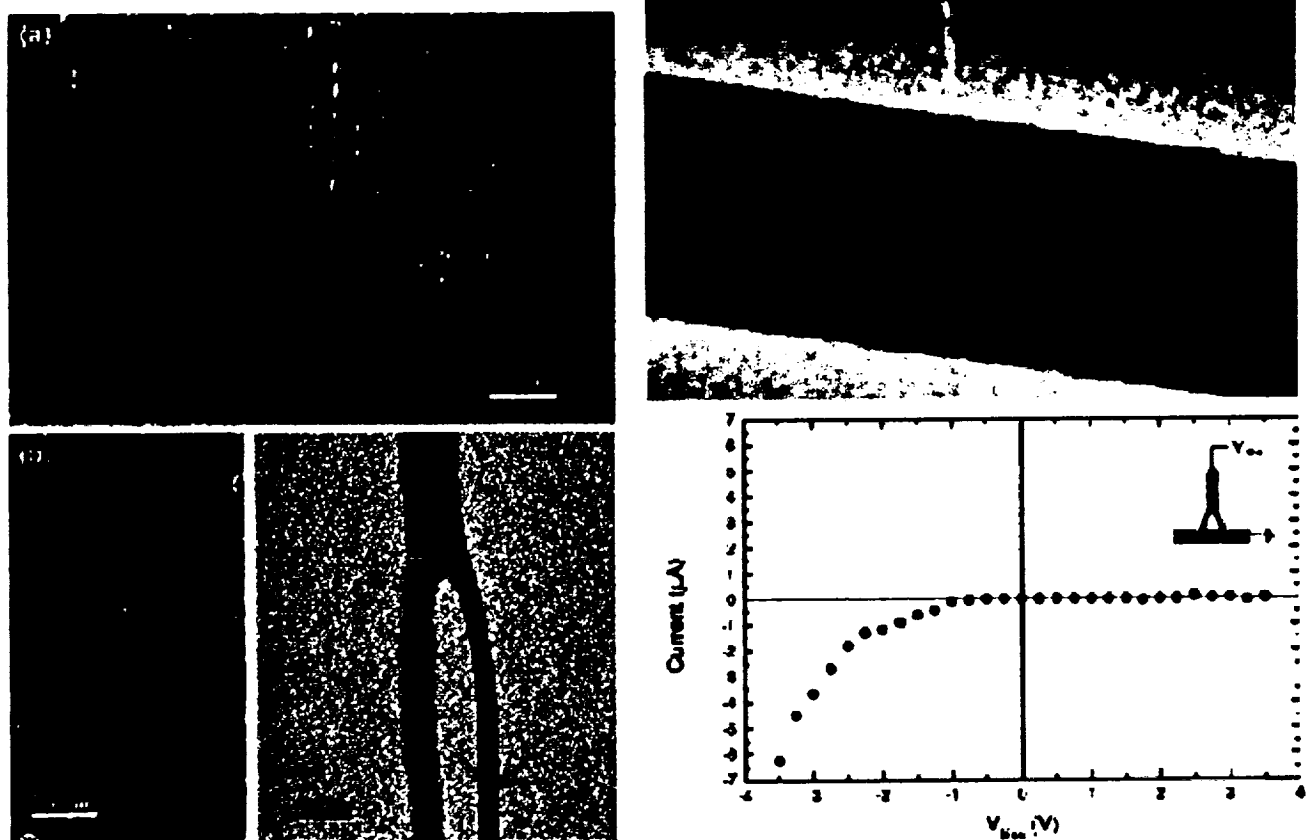
C. Papadopoulos,¹ A. Rukitin,¹ J. Li,¹ A. S. Vedenov,^{1,2} and J. M. Xu^{1,3}

¹*Department of Electrical & Computer Engineering, University of Toronto, 10 King's College Road, Toronto, Ontario, Canada M5S 3G4*

²*Russian Academy of Sciences, Institute of Radioengineering and Electronics, Fryazino, Moscow district 141120, Russia*

³*Division of Engineering, Brown University, Providence, Rhode Island 02912*

(Received 22 February 2000)



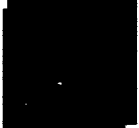
1st experimental Step to a Three-Terminal Nanoscale Transistor.



CNT in Microscopy

Atomic Force Microscopy is a powerful technique for imaging, nanomanipulation, as platform for sensor work, nanolithography...

Conventional silicon or tungsten tips wear out quickly. CNT tip is robust, offers amazing resolution.


100 nm wide, 40 nm high nanowire

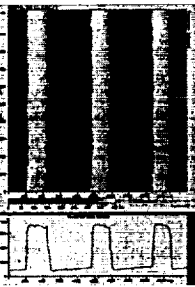
Simulated AFM image

10 nm

WWW.NANO.GOV

NASA Ames Research Center
Ramsey Stevens, Lance Delzeit, Cattien Nguyen

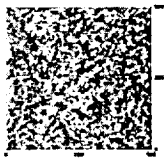
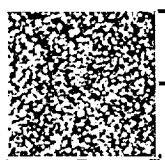
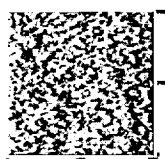
280 nm Line/Space Array of Polymeric Resist on silicon Substrate

Silicon Tip

Multi-Walled Carbon Nanotube Tip

AFM Imaging with Single Wall Nanotube Tips

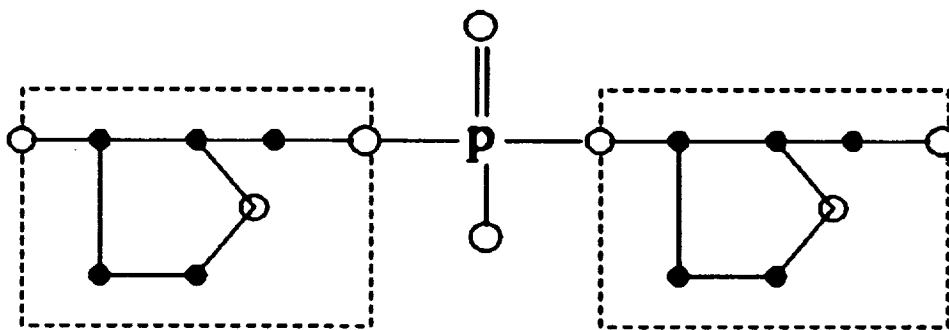




5 nm thick Ir on Mica

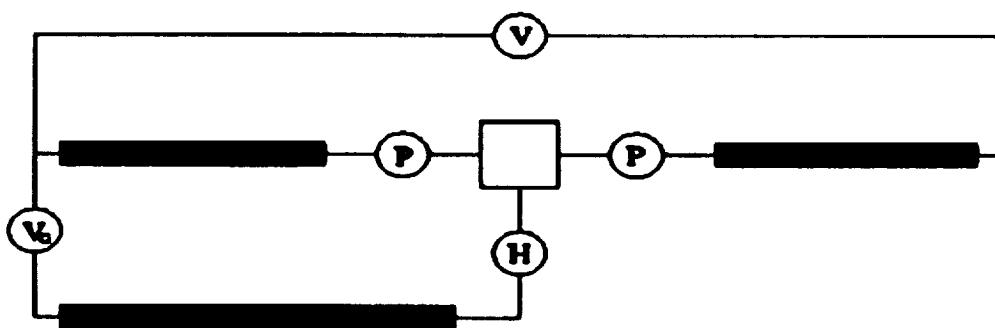
2 nm thick Au on Mica

Si₃N₄ on Silicon substrate

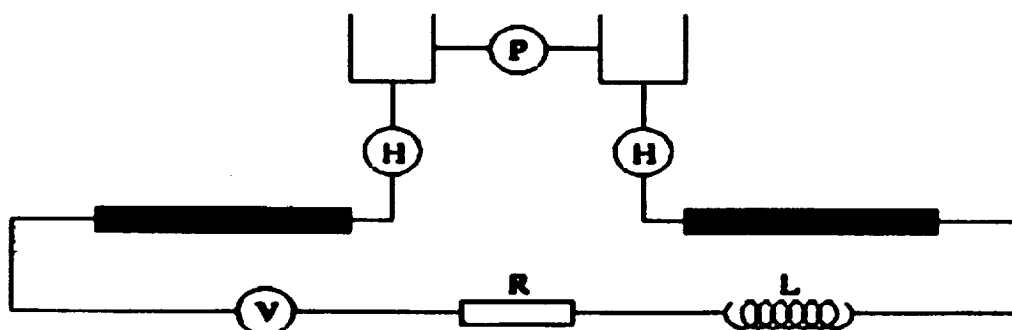
- Based on Phosphate bridges acting as tunnel junctions and H acting as capacitive element.
- DNA coated with metals can act as interconnects
- DNA has self-assembly properties



DNA Junctions



Single Electron Transistor

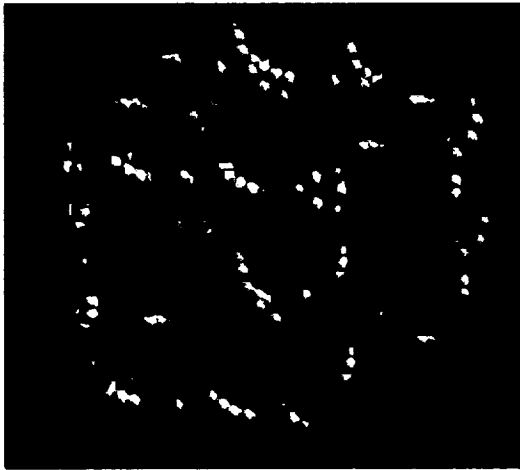


Quantum Bit

Example:

(NYU)

Topologically Connected DNA Segments



Cube



Truncated Octahedron

DAE



DAO



DPE



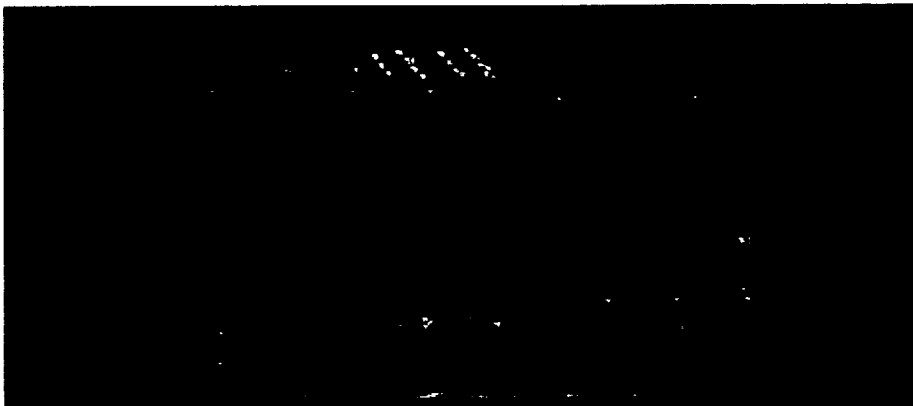
DPON



DPOW



**Double Cross-Over
Molecules**



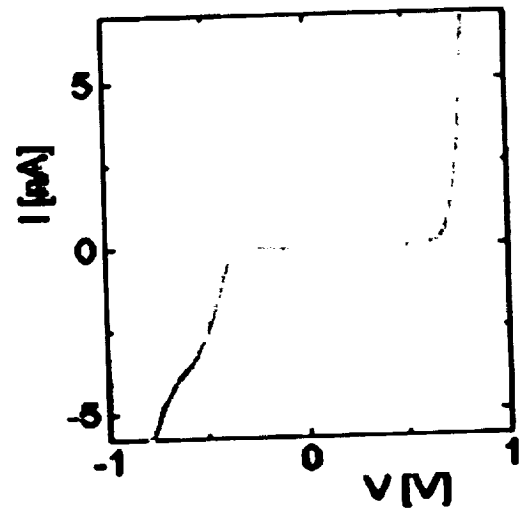
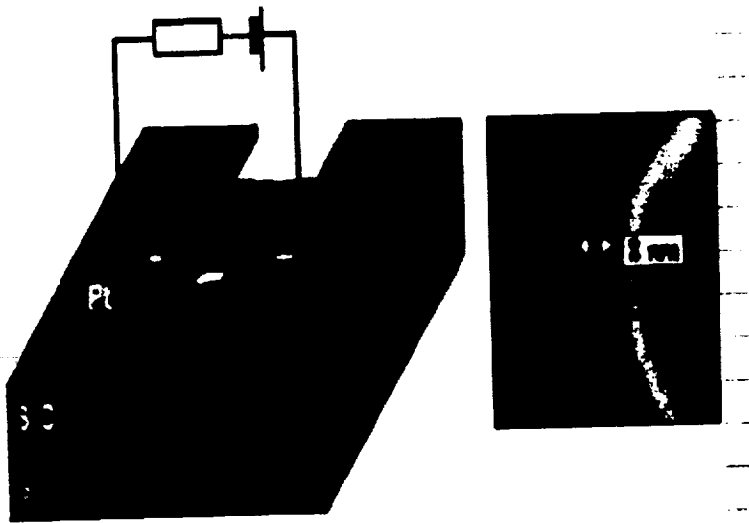
**DNA
Nano-mechanical
Device**

DNA as Electronics Elements:

Conflicting Claims about DNA as metal or semiconductor ?

Indirect measurements in the beginning led to this controversy?

Transport measurements on single DNA molecules C. Dekker (Delft)
Nature, 2000



A 10.4 nm long, double-stranded poly(G)–poly(C) DNA molecule
Metal nanoelectrodes that are separated by 8 nm

Small gap semiconductor

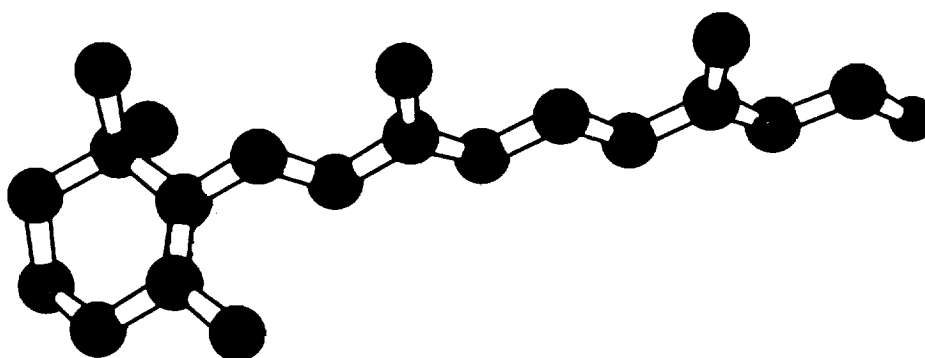
- Metal coated DNA serve as conductor.

Bacteriorhodopsin for Optical Data Storage

**Ann Hermone and Richard Jaffe
ahermone@mail.arc.nasa.gov**

- **Bacteriorhodopsin (BR) contains the chromophore retinal in an all-trans conformation.**
- **on photoexcitation retinal isomerizes from all-trans to mainly 13-cis.**
- **Changes in BR's optical properties in the excited state, such as refractive index, make it a candidate for optical data storage.**

All-trans Retinal



- **The lifetime of 13-cis retinal is short and when retinal returns to the all-trans form any data stored is lost.**
- **Mutant BR molecules have been prepared, in which retinal isomerizes to the 9-cis form with a long lifetime, making long-term data storage possible.**
- **Therefore, we are trying to characterize the 9-cis isomerization pathway.**

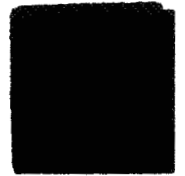


Nanotechnology: Comments

- Various experimental and simulation aspects of Nanoelectronics are currently in progress
- Individual devices and characteristics need to be incorporated in NASA specific applications
- Biosensors and nanotubes for interconnects are preliminary step in that direction



Nano-Electronics and Bio-Electronics



**Deepak Srivastava
NASA Ames Research Center
MS T27A-1 and MS 229-3
Moffett Field, CA 94034-1000**

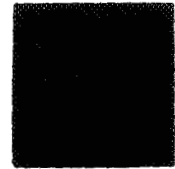
deepak@nas.nasa.gov, (650) 604-3486

<http://www.ipt.arc.nasa.gov>

<http://www.nas.nasa.gov/~deepak/home.html>



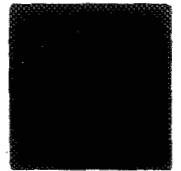
Why Nanotechnology at NASA?



- **Advanced miniaturization, a key thrust area to enable new science and exploration missions**
 - **Ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed**
- **Revolutions in electronics and computing will allow reconfigurable, autonomous, "thinking" spacecraft**
- **Nanotechnology presents a whole new spectrum of opportunities to build device components and systems for entirely new space architectures**
 - **Networks of ultrasmall probes on planetary surfaces**
 - **Micro-rovers that drive, hop, fly, and burrow**
 - **Collection of microspacecraft making a variety of measurements**



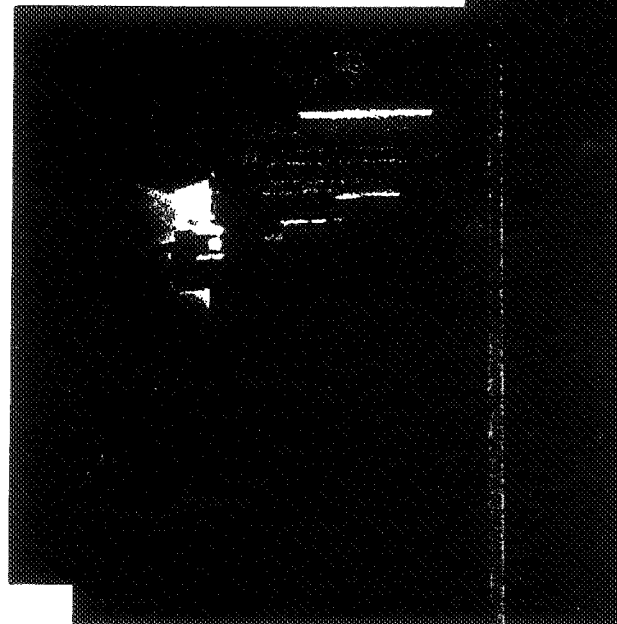
NASA Ames Nanotechnology Program



- **Started in FY 97, currently about 25 FTEs on site working on nanotechnology research: additional 15 FTEs involved in simulation, process modeling, and computational chemistry**
- **Research focus ranges from carbon and protein nanotubes, quantum device physics, quantum computing, data storage to optoelectronics, DNA electronics, Bio-Sensors, Bacteriorhodopsin based Data-Storage**
- **Largest carbon nanotube effort in the Federal government and also one of the largest in the world**
 - **About ~60 refereed publications in the field**
 - **Over 100 talks in National/International Meetings**
 - **Two Feynmann Awards**

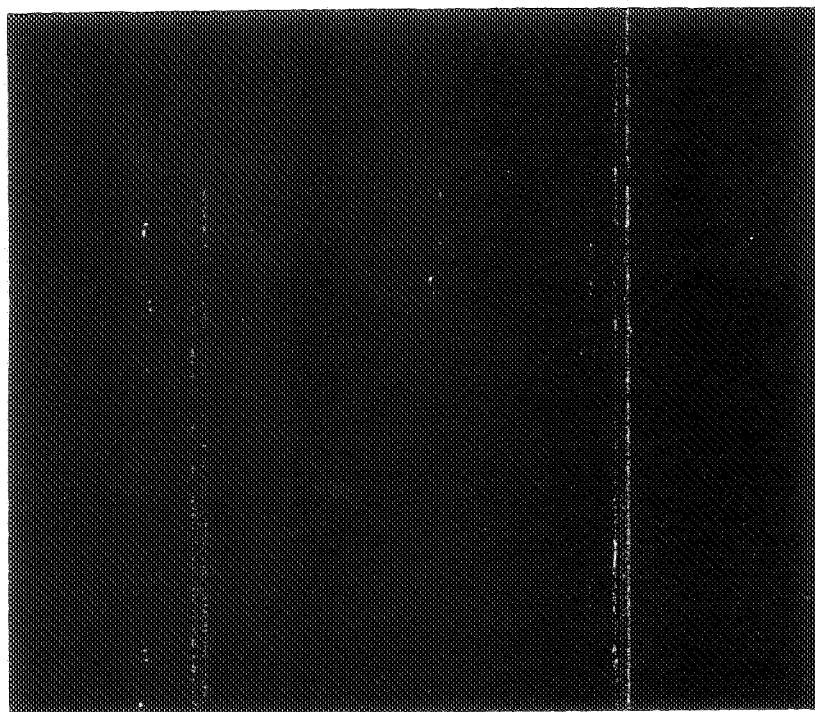
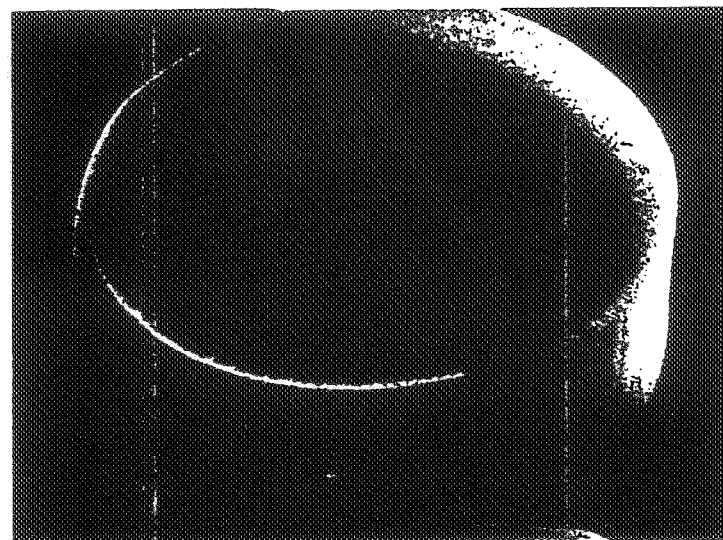
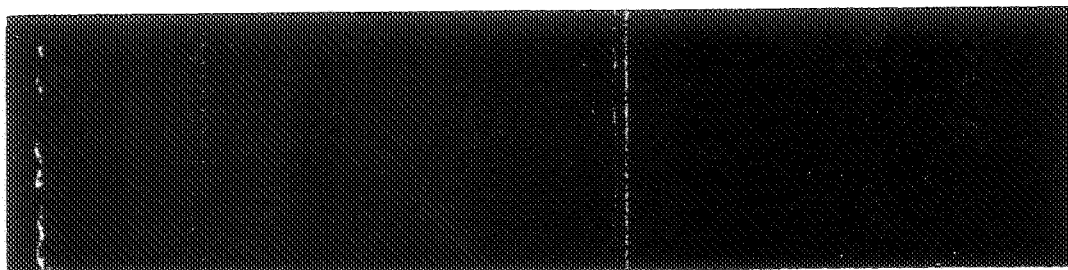
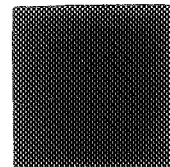
CNT Synthesis

- CNT has been grown by laser ablation (pioneering at Rice) and carbon arc process (NEC, Japan) - early 90s.
 - SWNT, high purity, purification methods
- CVD is ideal for patterned growth (electronics, sensor applications)
 - Well known technique from microelectronics
 - Hydrocarbon feedstock
 - Growth needs catalyst (transition metal)
 - Multiwall tubes at 500-800° deg. C.
 - Numerous parameters influence CNT growth

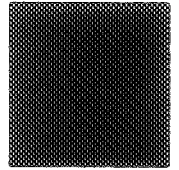




Carbon Nanotubes at Ames

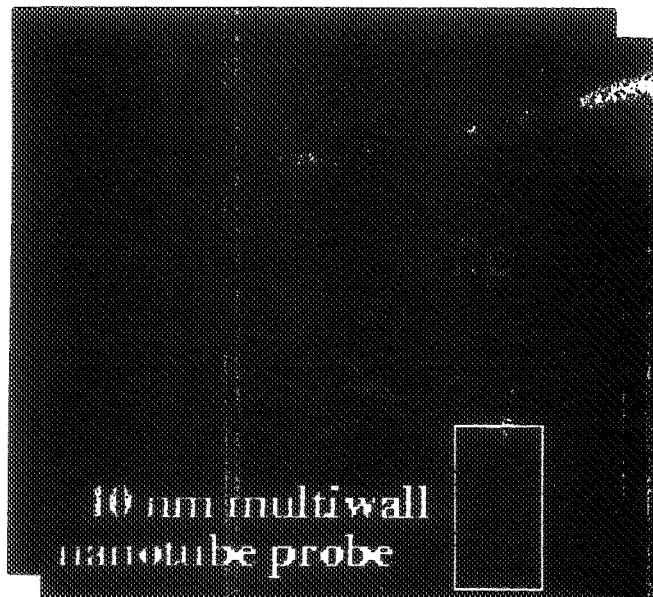


CNT in Microscopy

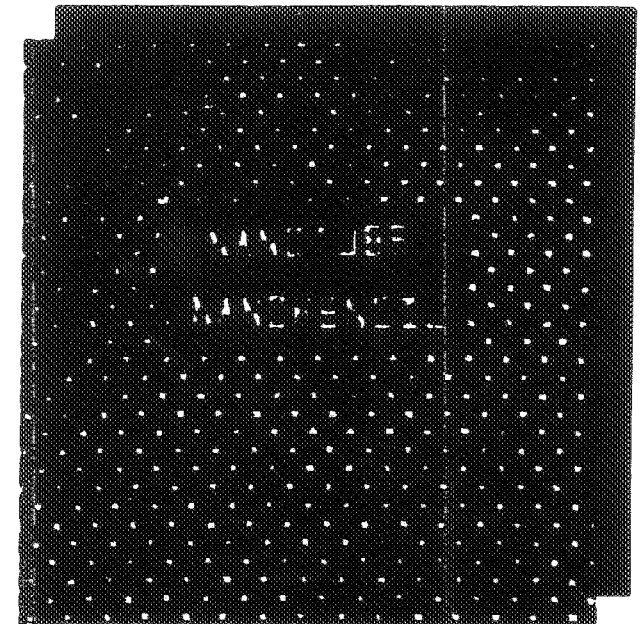
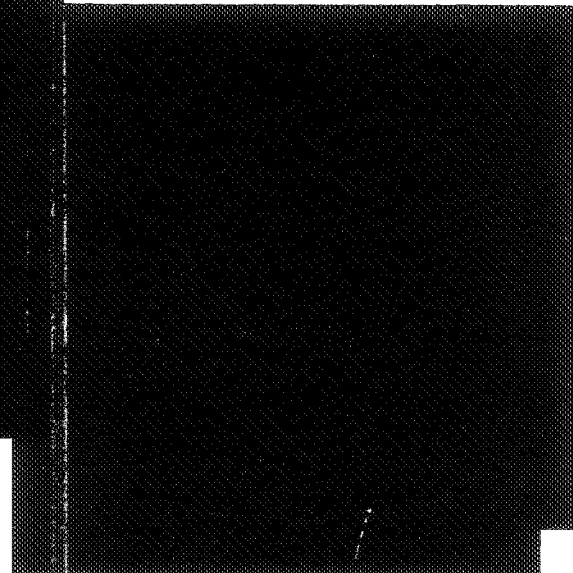


Atomic Force Microscopy is a powerful technique for imaging, nanomanipulation, as platform for sensor work, nanolithography...

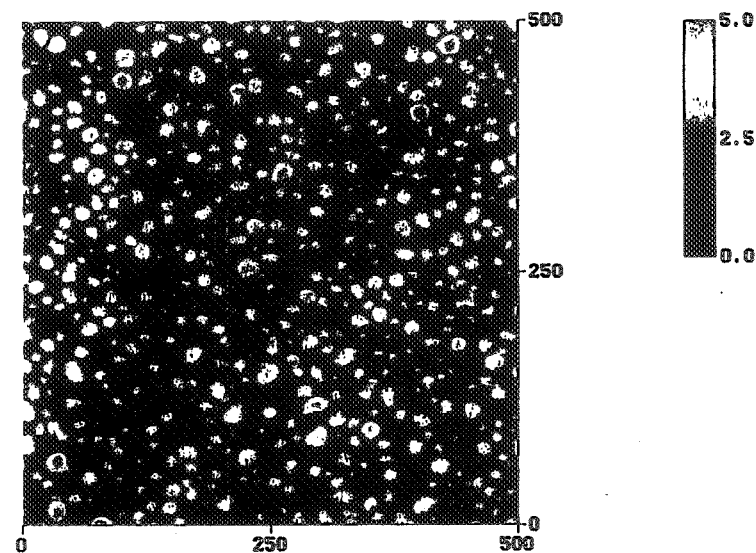
Conventional silicon or tungsten tips wear out quickly. CNT tip is robust, offers amazing resolution.



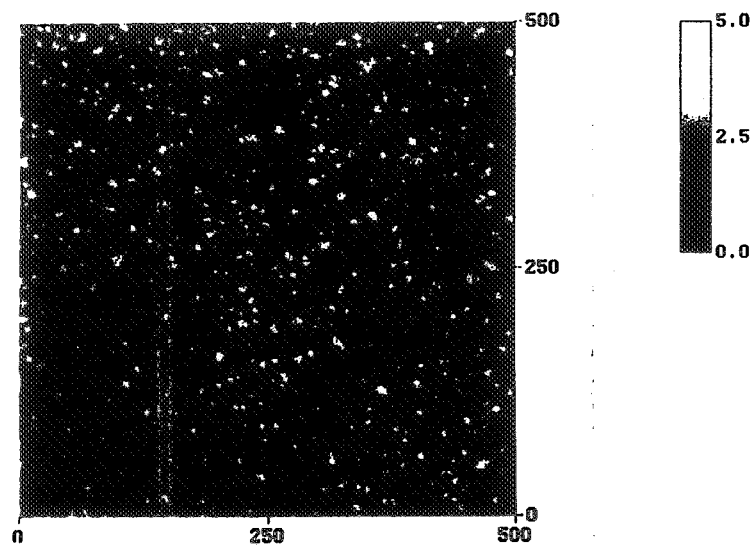
Simulated Mars dust



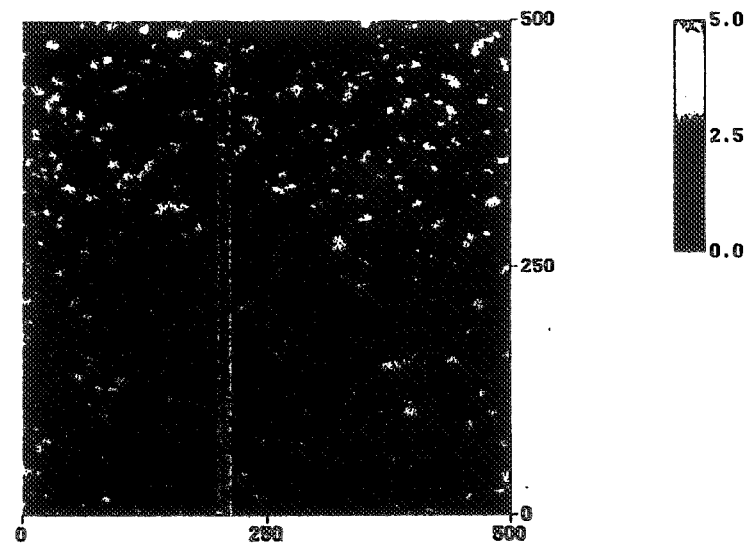
AFM Imaging with Single Wall Nanotube Tips



2 nm thick Au on Mica

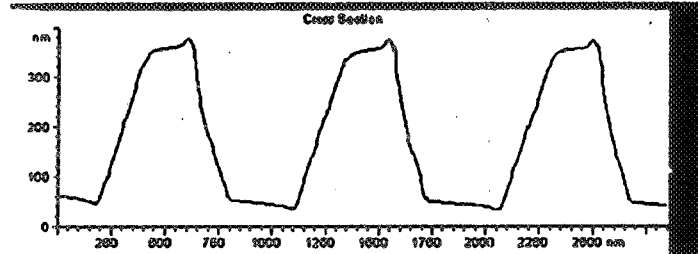
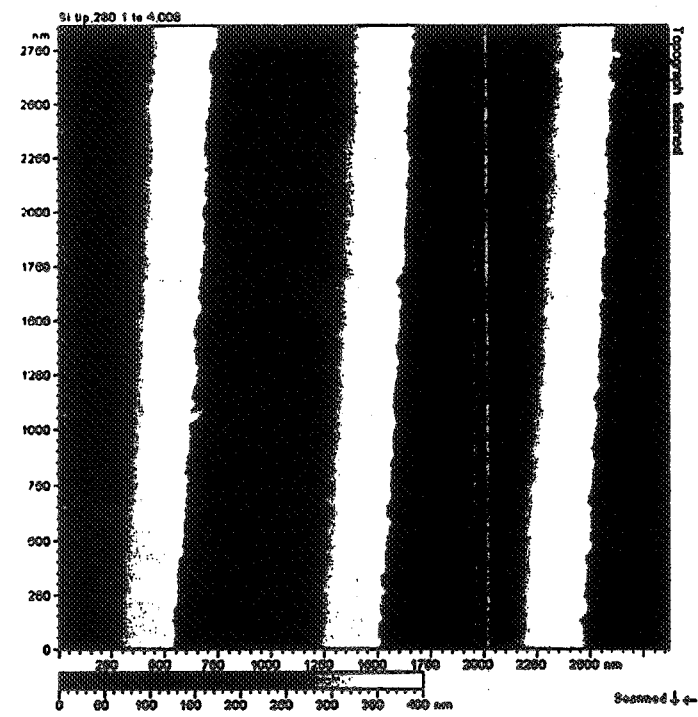


5 nm thick Ir on Mica

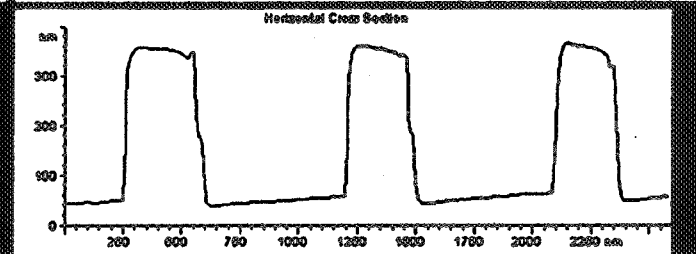
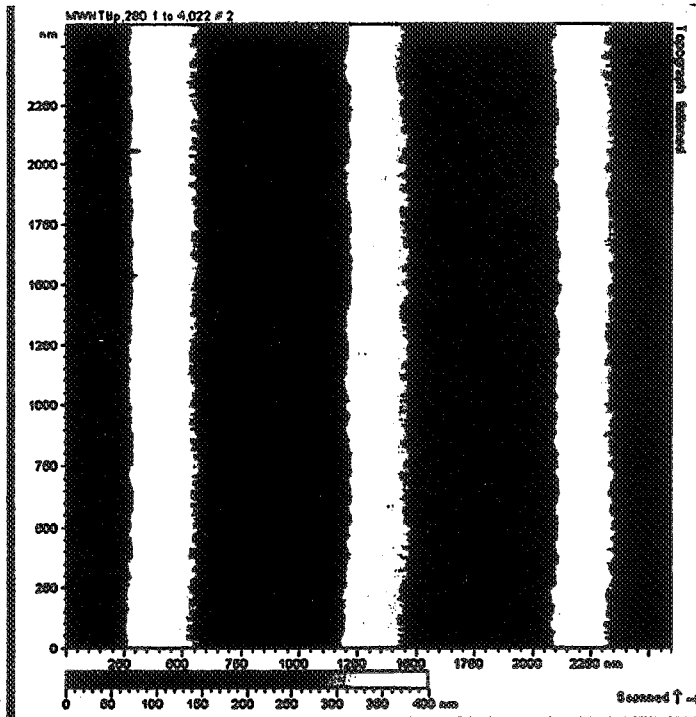


Si_3N_4 on Silicon substrate

280 nm Line/Space Array of Polymeric Resist on silicon Substrate



Silicon Tip

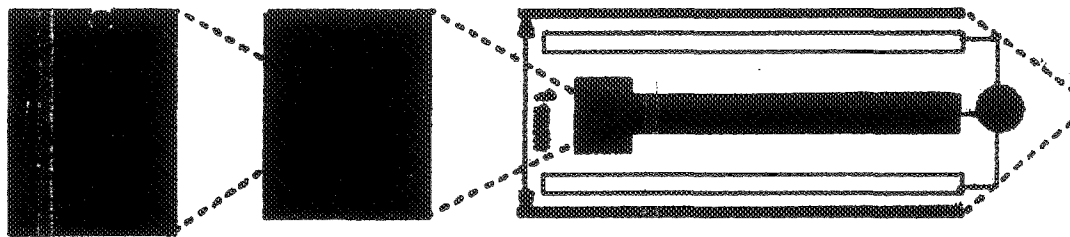


Multi-Walled Carbon
Nanotube Tip

CNT Based Biosensors

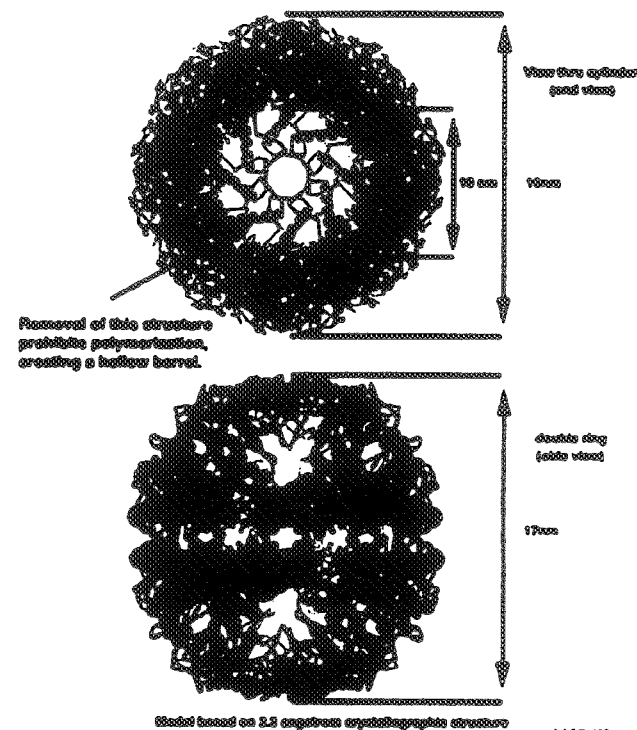
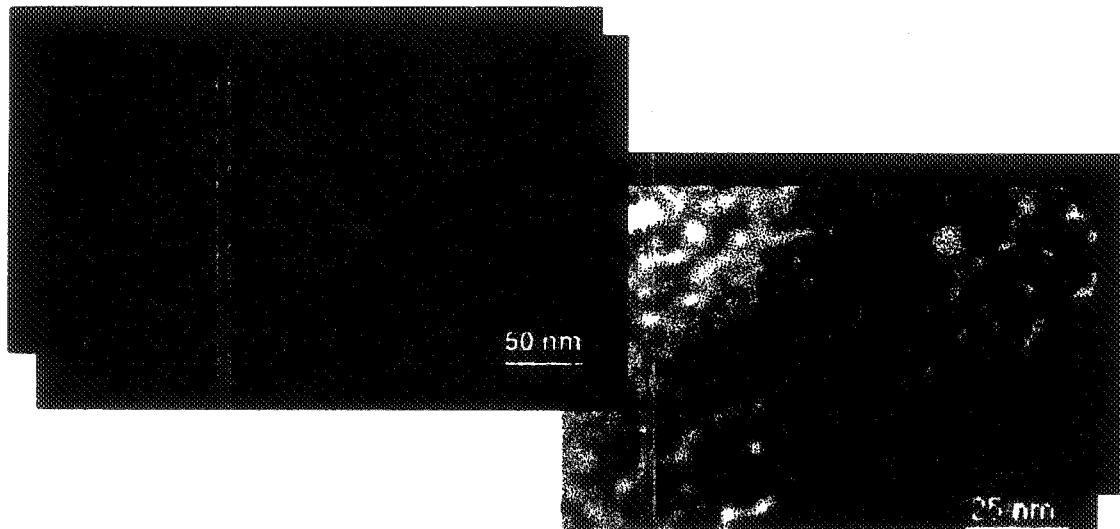
- Our interest is to develop sensors for astrobiology to study origins of life. CNT, though inert, can be functionalized at the tip with a probe molecule. Current study uses AFM as an experimental platform.
- The technology is also being used in collaboration with NCI to develop sensors for cancer diagnostics
 - Identified probe molecule that will serve as signature of leukemia cells, to be attached to CNT
 - Current flow due to hybridization will be through CNT electrode to an IC chip.
 - Prototype biosensors catheter development

- High specificity
- Direct, fast response
- High sensitivity
- Single molecule and cell signal capture and detection

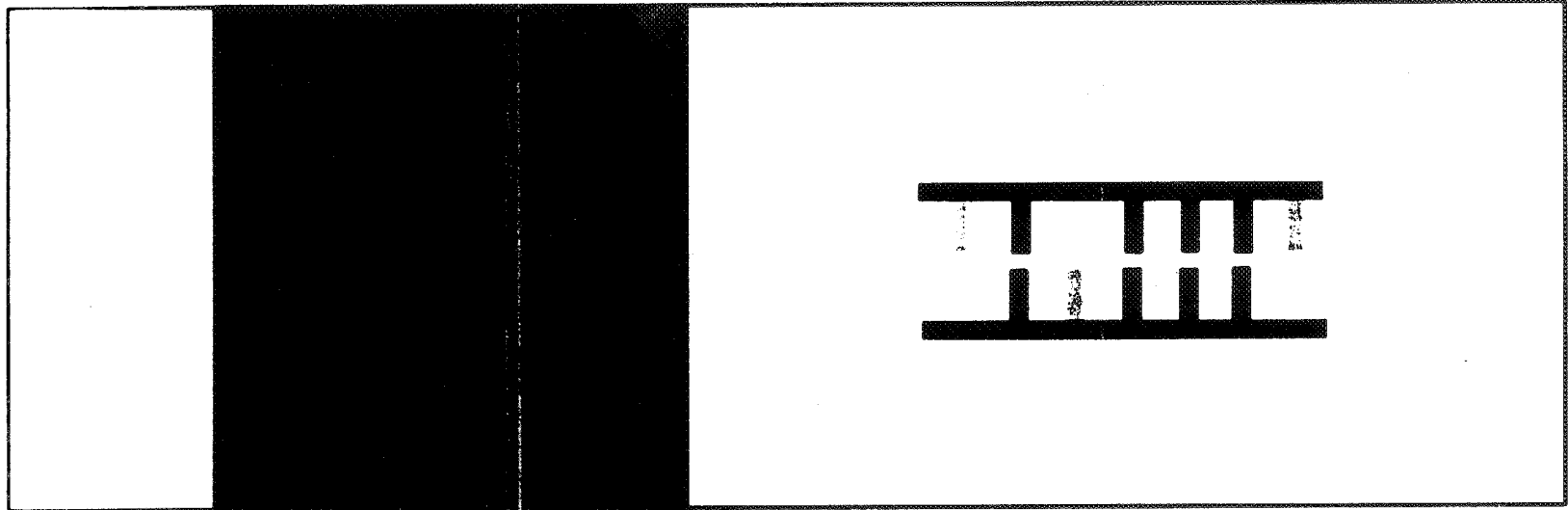


Protein Nanotubes

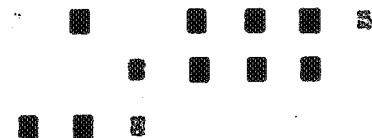
- Heat shock protein (HSP 60) in organisms living at high temperatures (“extremophiles”) is of interest in astrobiology
- HSP 60 can be purified from cells as a double-ring structure consisting of 16-18 subunits. The double rings can be induced to self-assemble into nanotubes.



IMPORTANCE

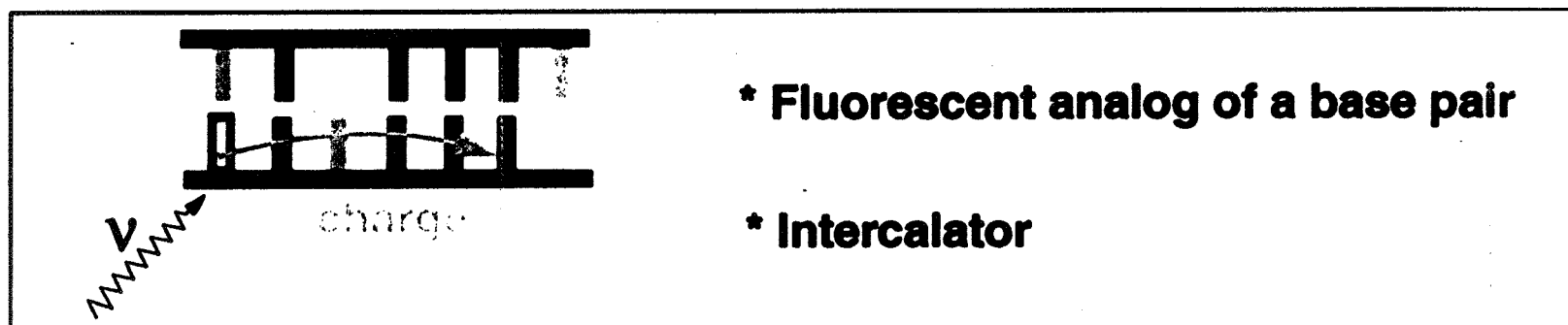


- **Conductivity of DNA has been controversial for decades.**
- **Electron transfer experiments (biochemistry) / Possible connection to cancer**
- **Transport experiments (physics)**
- **DNA Electronics (Device / Lithography)**

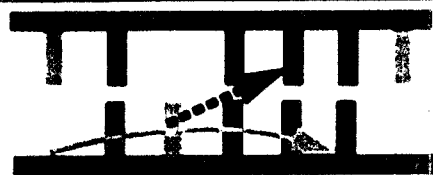


ELECTRON TRANSFER EXPERIMENTS

- Oxidative damage of DNA has been linked to cancer.
- How effective is long range electron transfer in causing oxidative damage?

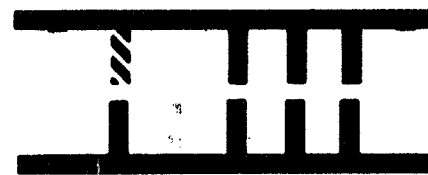


- Estimates of electron transfer rates span two orders of magnitude.



Intrastrand & Interstrand

Significant dependence
on intervening sequence



Significant dependence
on base pair mismatches.

TRANSPORT EXPERIMENTS

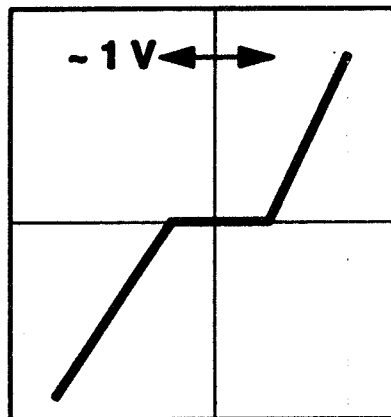
Voltage



Porath et. al, Nature (2000)

INSULATING

Current
~ 1 nA

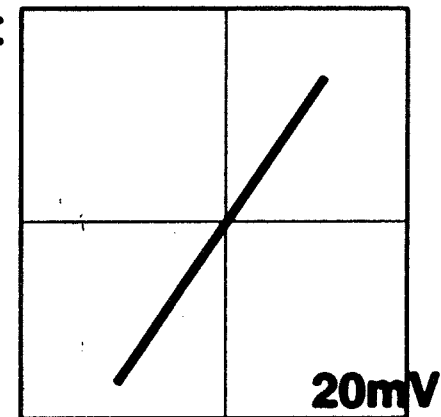


Voltage (V)

Fink et. al, Science (1999)

NO GAP!

Current
~ 10 nA

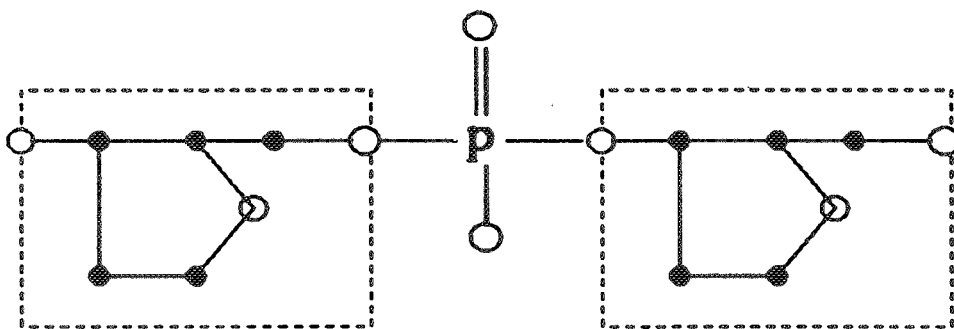


Voltage (mV)

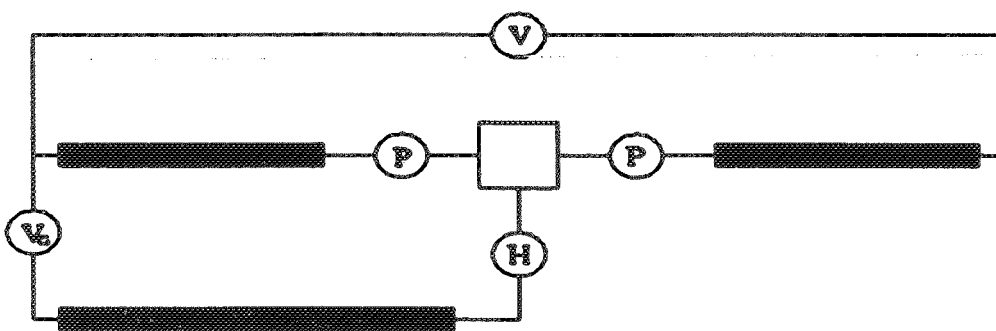
Based on Phosphate bridges acting as tunnel junctions and H acting as capacitive element.

DNA coated with metals can act as interconnects

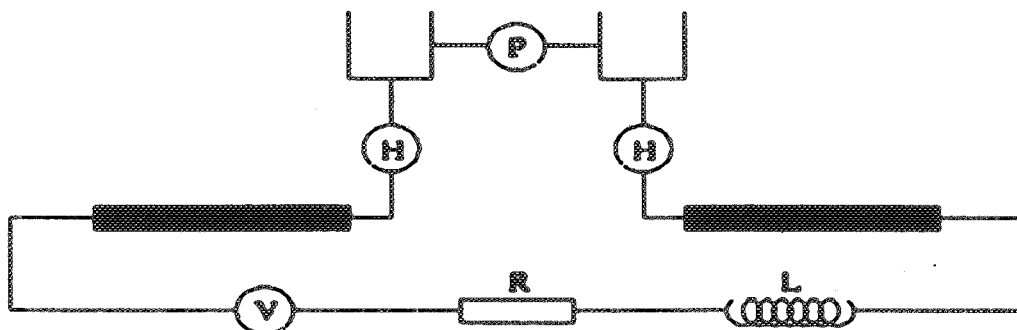
DNA has self-assembly properties



DNA Junctions



Single Electron Transistor



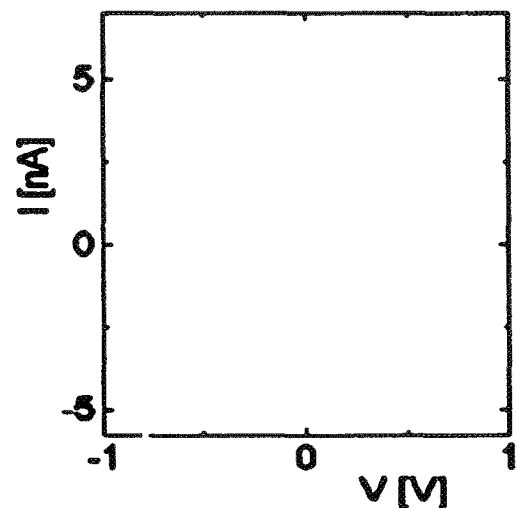
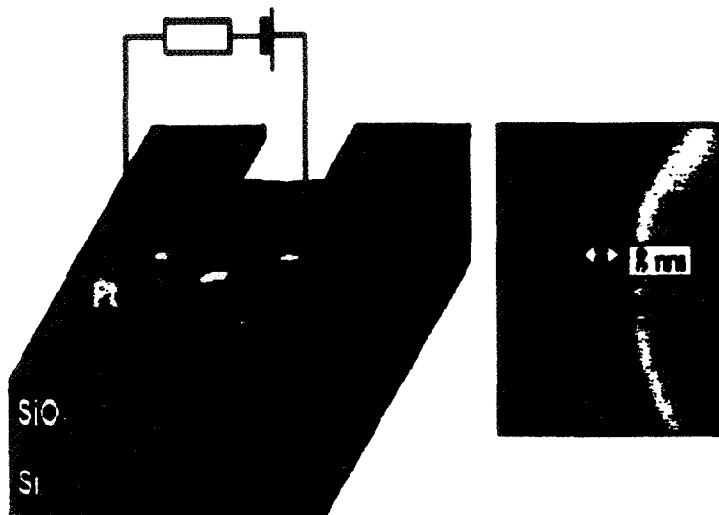
Quantum Bit

DNA as Electronics Elements:

about DNA as metal or semiconductor ?

Indirect measurements in the beginning led to this controversy?

Transport measurements on single DNA molecules C. Dekker (Delft)
Nature, 2000



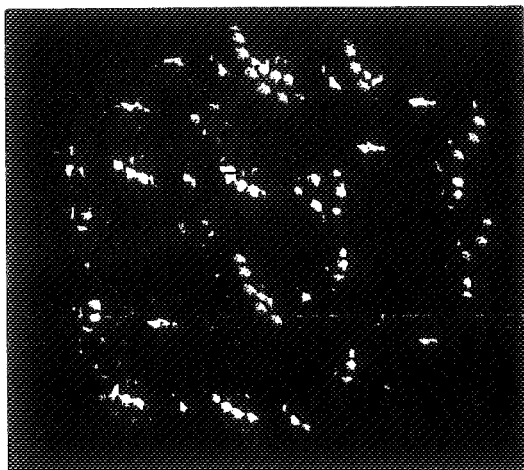
A 10.4 nm long, double-stranded poly(G)–poly(C) DNA molecule
Metal nanoelectrodes that are separated by 8 nm

Source: <http://www.nature.com/nature>

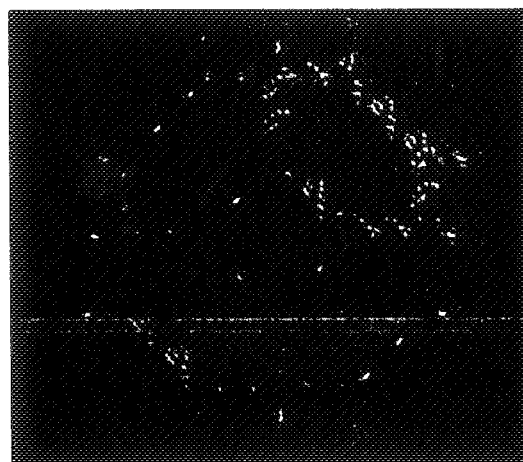
Metal coated DNA serve as conductor.

Example:

(NYU)



Cube



Truncated Octahedron

DAE

DAO

DPE

DPON

DPOW

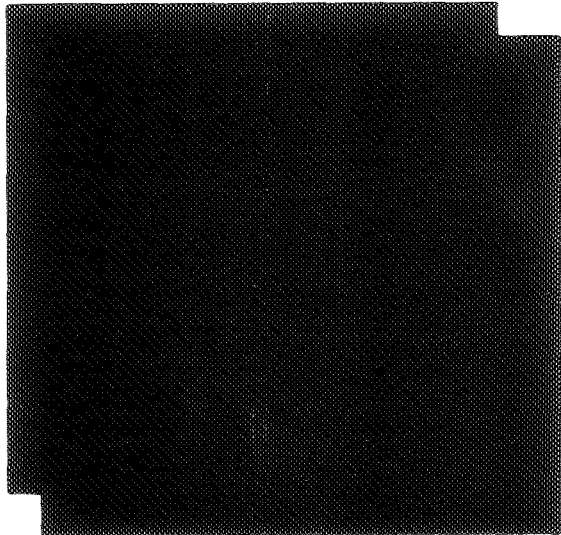


**Double Cross-Over
Molecules**

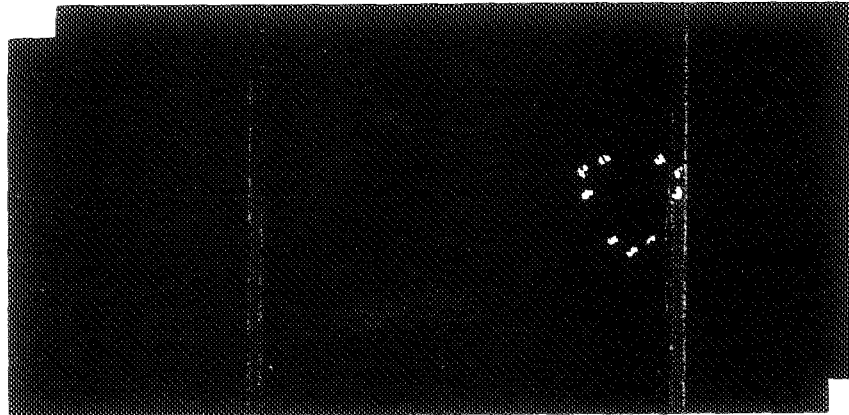


**DNA
Nano-mechanical
Device**

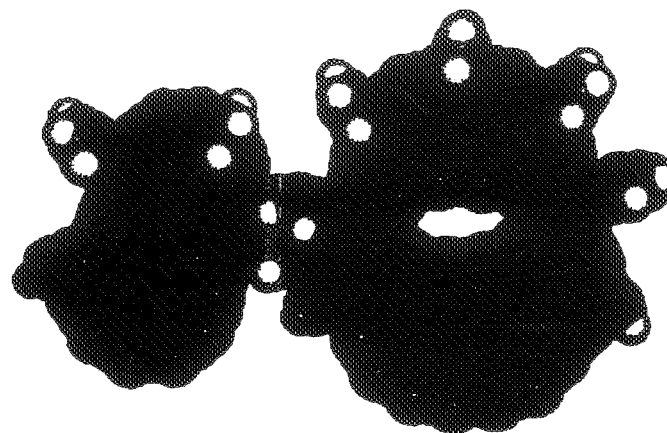
- Large scale computer simulations based on ab initio methods enable understanding nanotube characteristics and serve as design tool
 - Evaluation of mechanical properties
 - Evaluation of electronic properties
 - Electron transport in CNT devices
 - Functionalization of the nanotubes
 - Design of electrical and mechanical devices
 - Evaluation of storage potential (H_2 , Li)



CNT Molecular Network

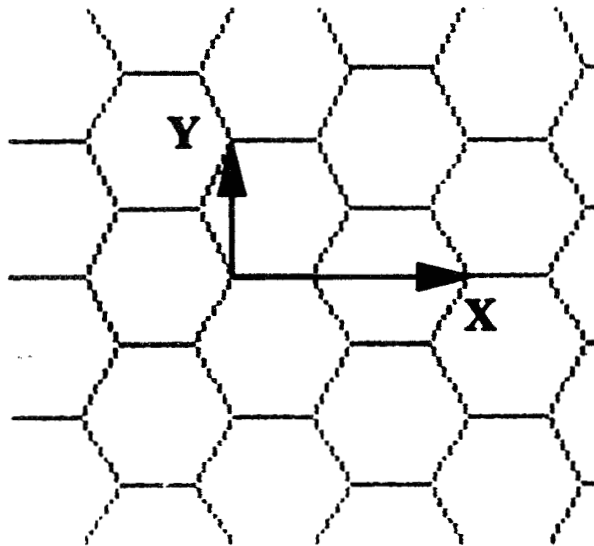


CNT 'T' and 'Y' Junctions

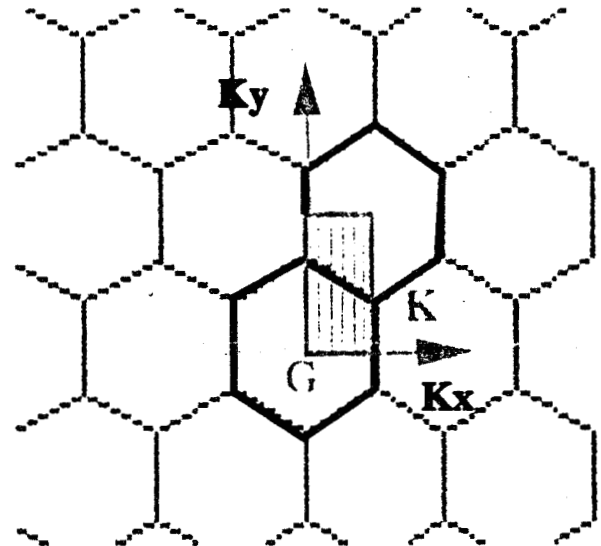




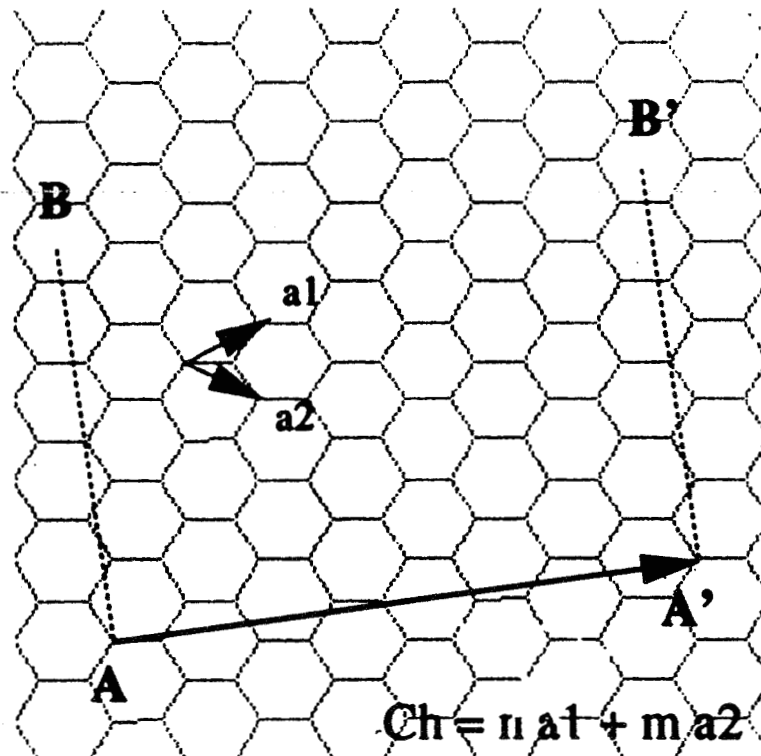
Carbon Nanotube Electronics Band Structure (basics)



Hexagonal Lattice of a Graphene Sheet – (2x unit cell)

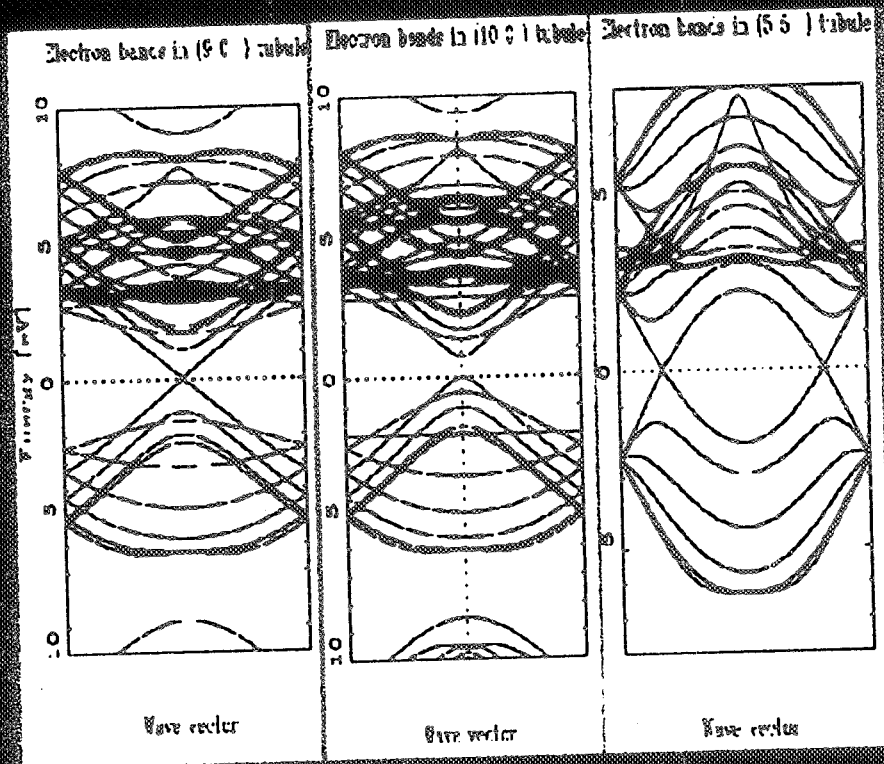
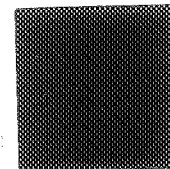


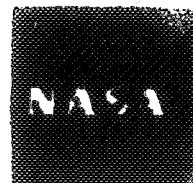
First Brillouin zone for an arm-chair tube.



$$\mathbf{Ch} = n \mathbf{a}_1 + m \mathbf{a}_2 \quad (\text{chiral vector})$$

Computational Nanotechnology





3-terminal CNT Heterojunctions

VOLUME 79, NUMBER 22

PHYSICAL REVIEW LETTERS

1 DECEMBER 1997

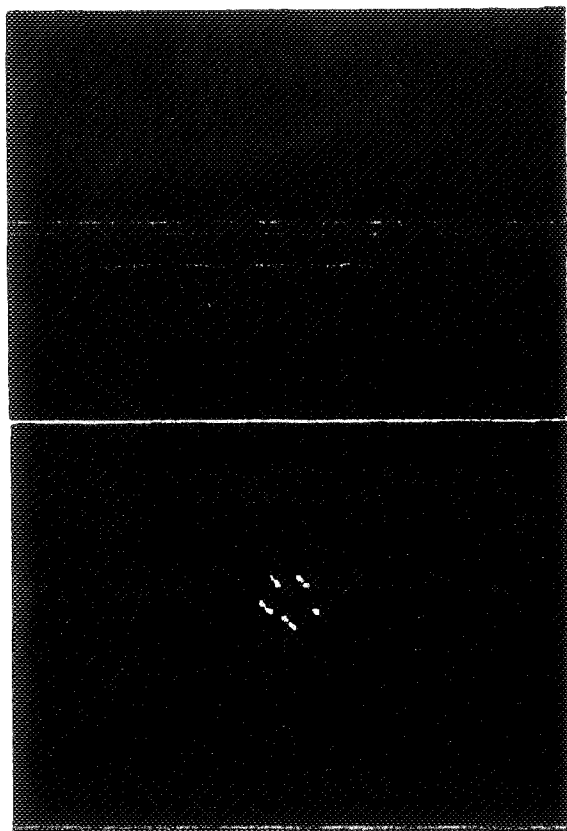


FIG. 1. (color). (a) Fully relaxed (5,5)-(10,0)-(5,5) tube (T1). The turquoise colored balls denote the atoms forming the heptagons. The structure contains six heptagons and no pentagons. (b) Fully relaxed (9,0)-(10,0)-(9,0) tube (T2). The turquoise colored balls denote the atoms forming the heptagons. Pentagons are denoted by white balls. The structure contains eight heptagons and two pentagons.

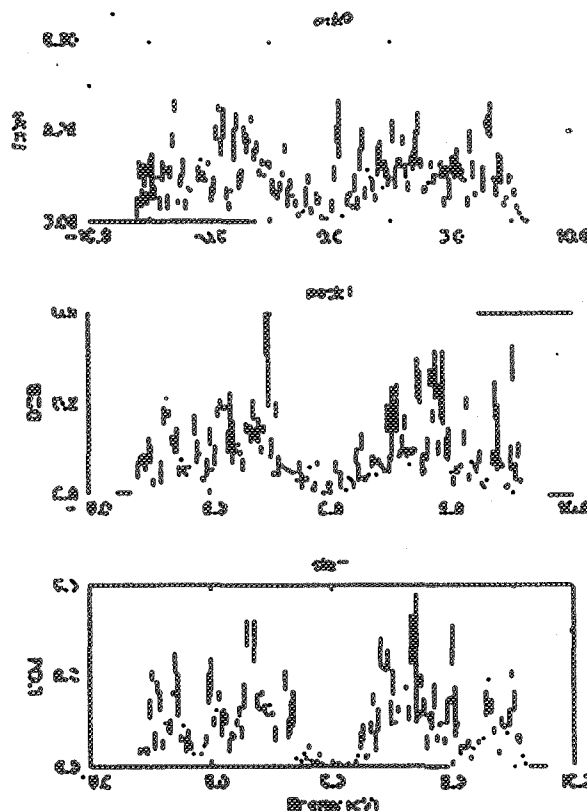
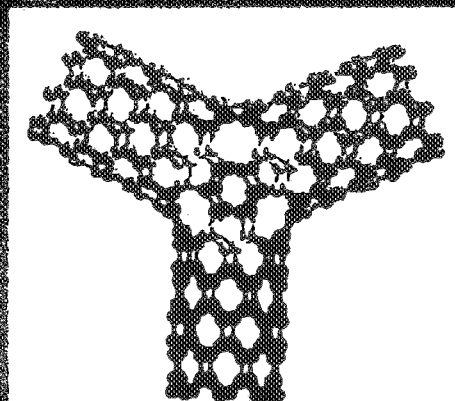
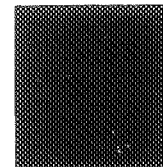


FIG. 3. LDOS for the relaxed (9,0)-(10,0)-(9,0) structure (T2) at various cross sections indicated in Fig. 1(b). The larger contribution in the gap is due to the presence of two extra pairs of heptagon-pentagon defects at the junction.

LDOS of (10,0)-(9,0) "T-junction"

3-terminal "T-tunnel" CNT Heterojunctions for Molecular Electronics Applications





Multi-wall Y-junction Carbon Nanotubes



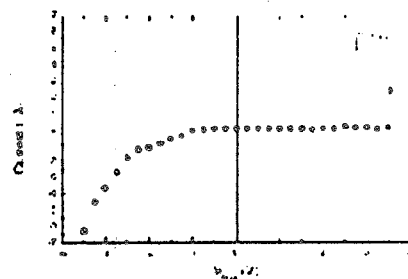
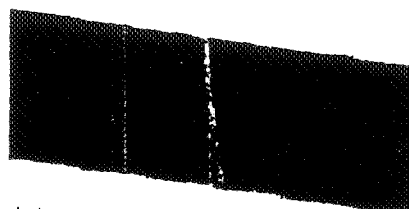
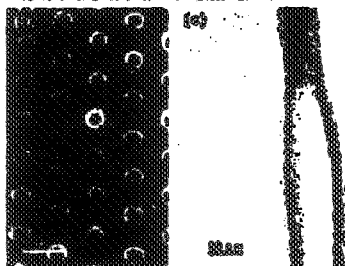
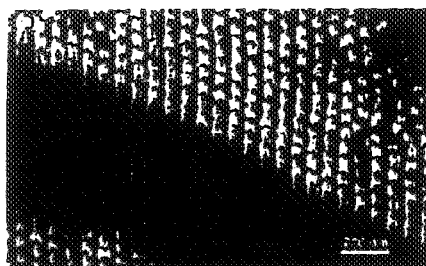
PHYSICAL REVIEW LETTERS

Electronic Transport in Y-Junction Carbon Nanotubes

C. Papadopoulos, A. Kulkarni, J. Li, V. S. Varshney, and J. M. Xu

Department of Electrical and Computer Engineering, University of Kentucky, Lexington, Kentucky 40506-0046, USA

Received 11 July 2000; accepted for publication 28 August 2000



PHYSICAL REVIEW LETTERS

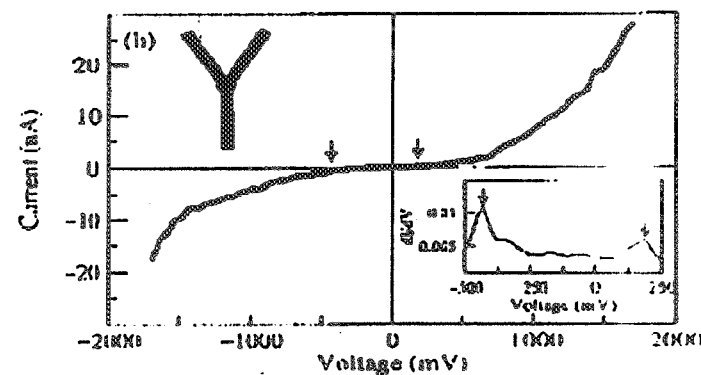
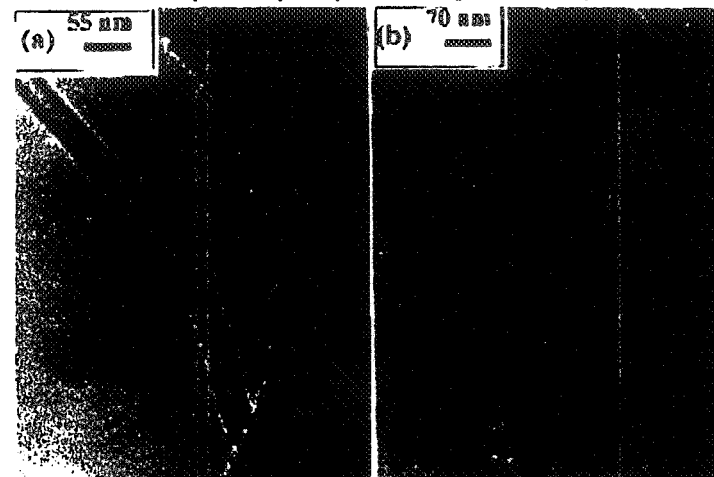
PHYSICAL REVIEW LETTERS

Y-junction carbon nanotubes

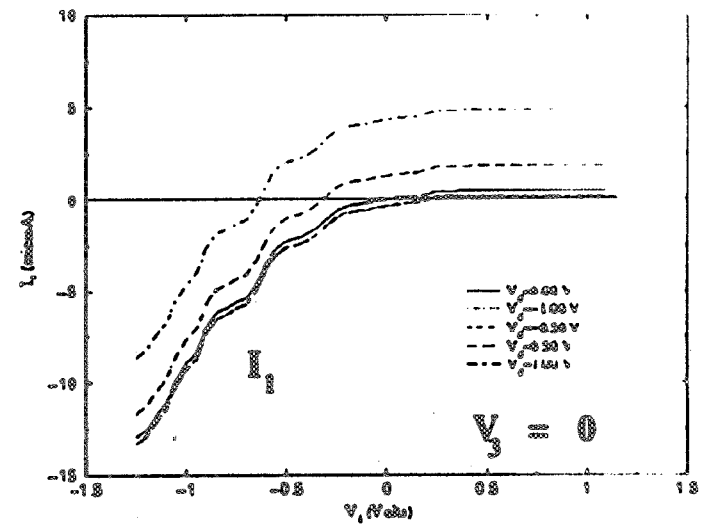
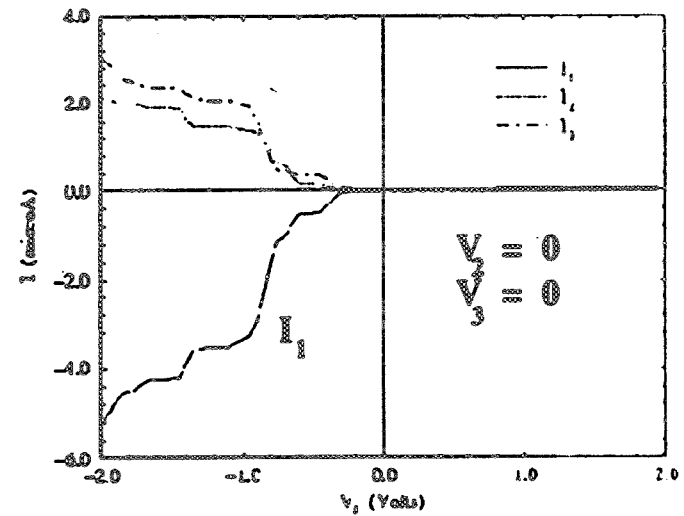
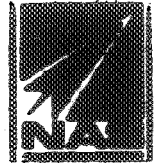
S. C. Saha, J. Li, J. M. Xu, A. Kulkarni, and C. N. S. Rao

Department of Electrical and Computer Engineering, University of Kentucky, Lexington, Kentucky 40506-0046, USA

Received 11 July 2000; accepted for publication 28 August 2000



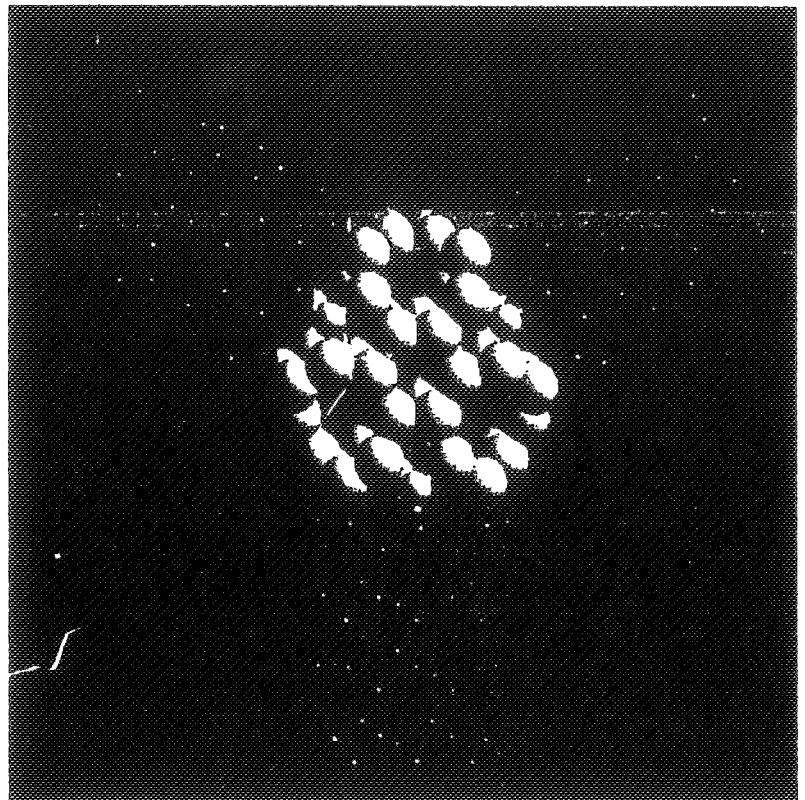
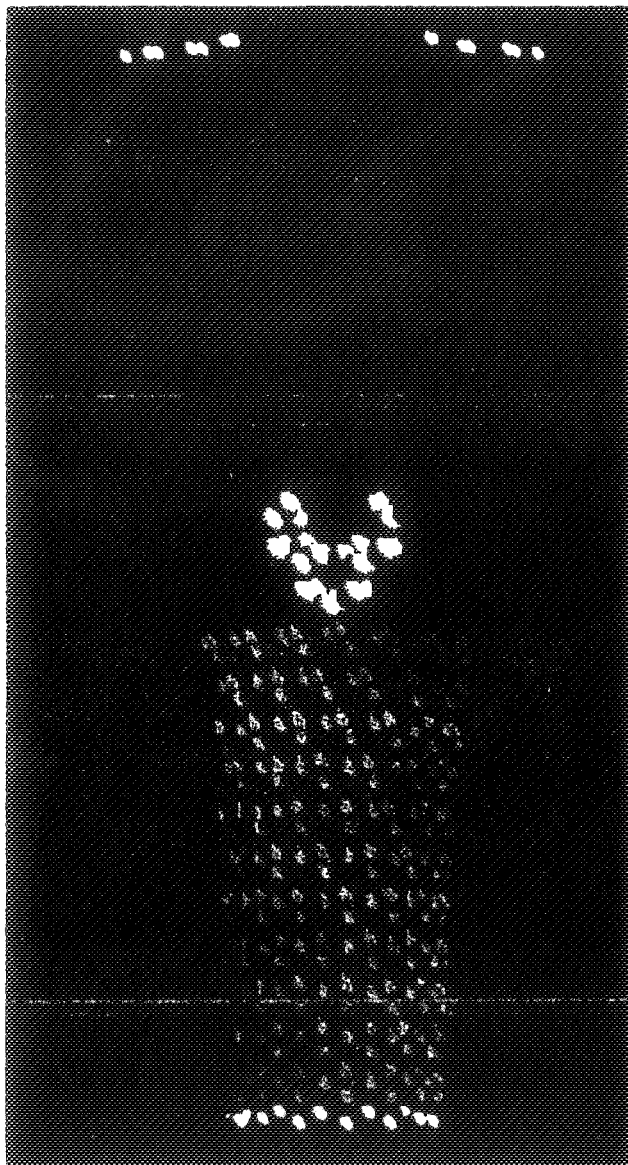
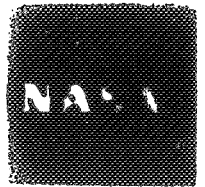
NASA



A Andriotis, M. Menon, D. Srivastava and, L. Chernozatonski, submitted, Phys. Rev. Lett. (2001)

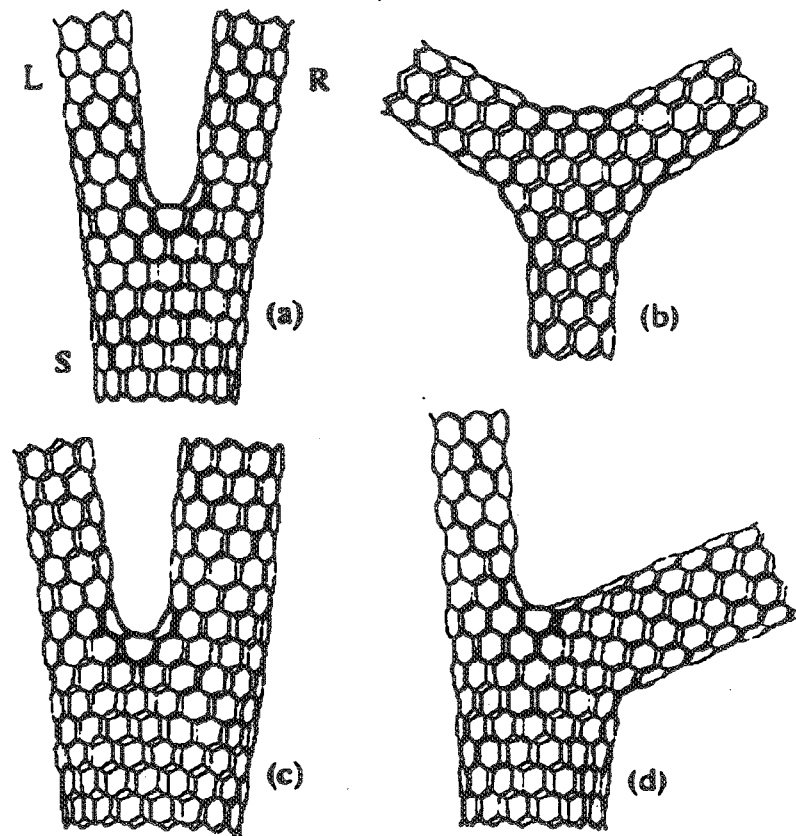
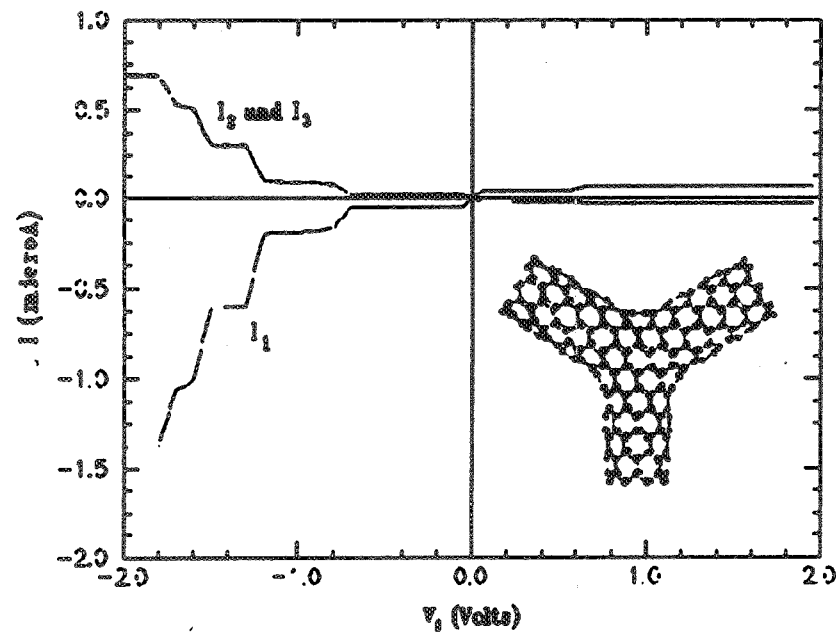


Semiconducting Y-junction Nanotubes with Different Angles



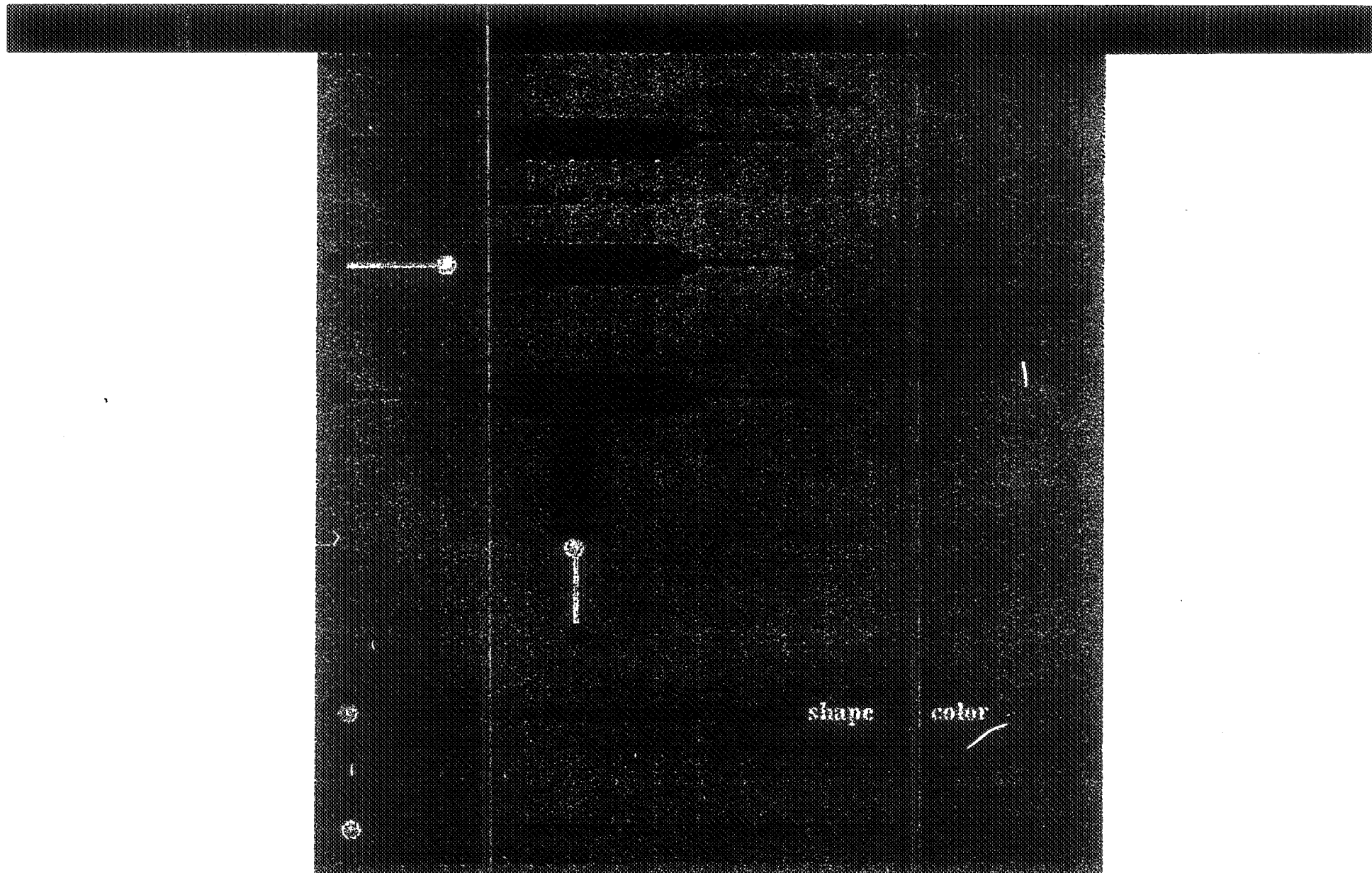
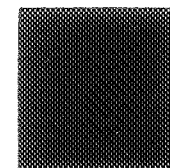
Ballistic Room

Temperature

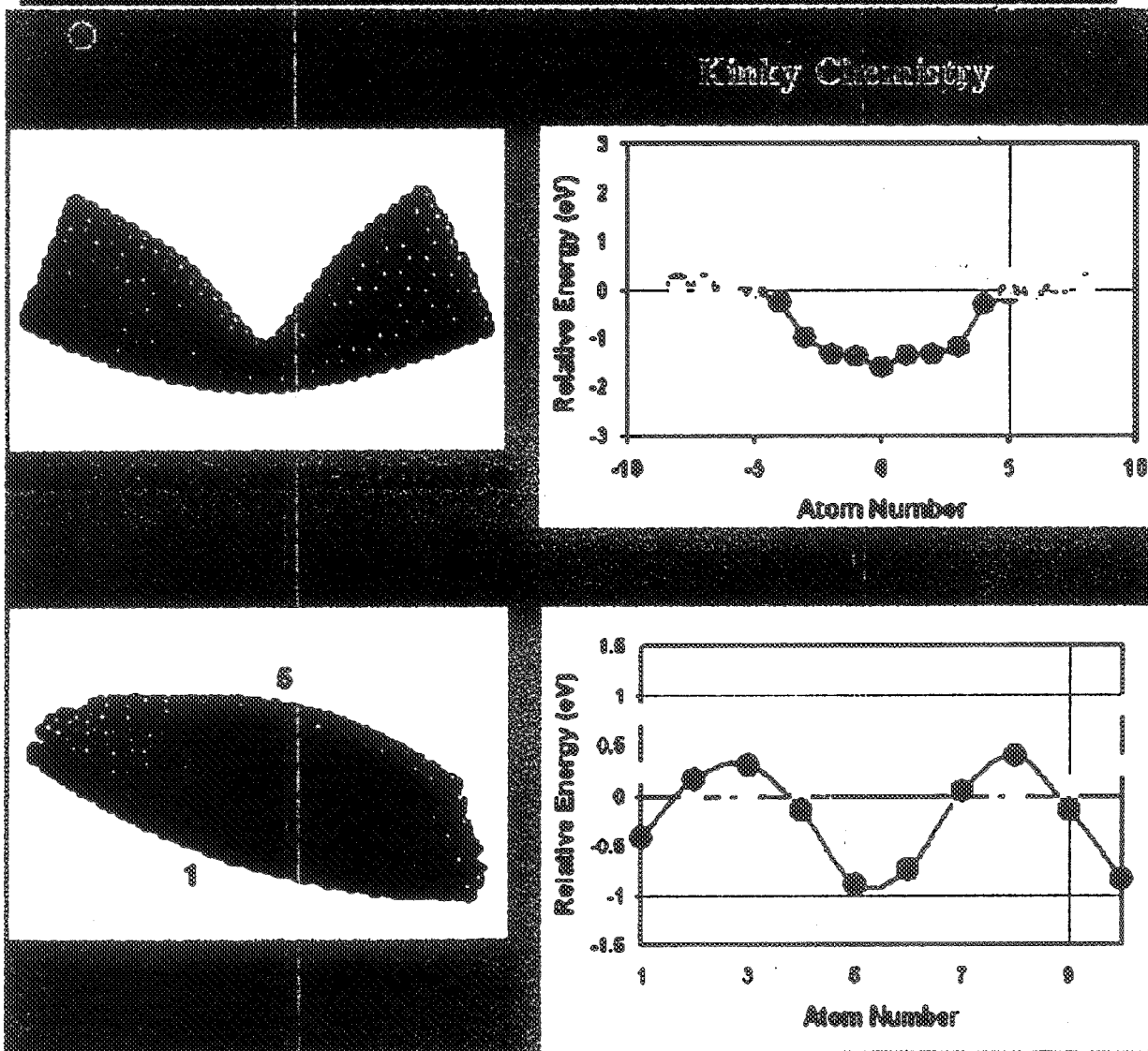


A Andriotis, M. Menon, D. Srivastava and L. Chernozatonski,
submitted, Appl. Phys. Lett. (2001)

Computational Nanotechnology



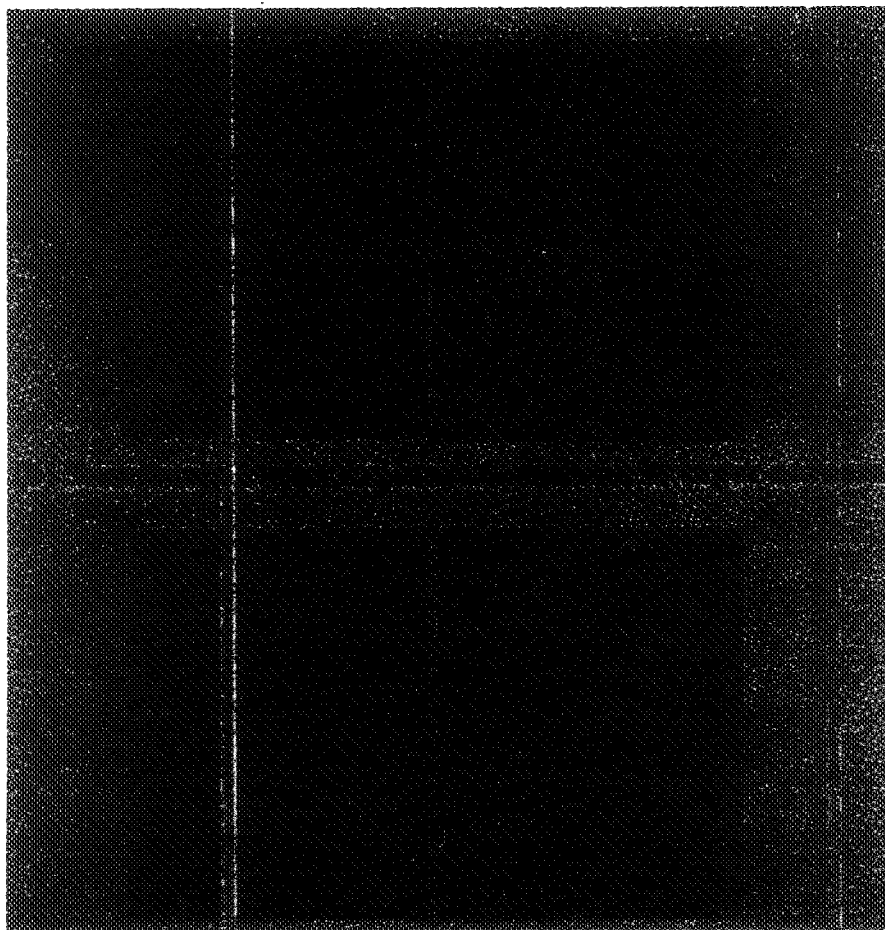
Kinky Chemistry



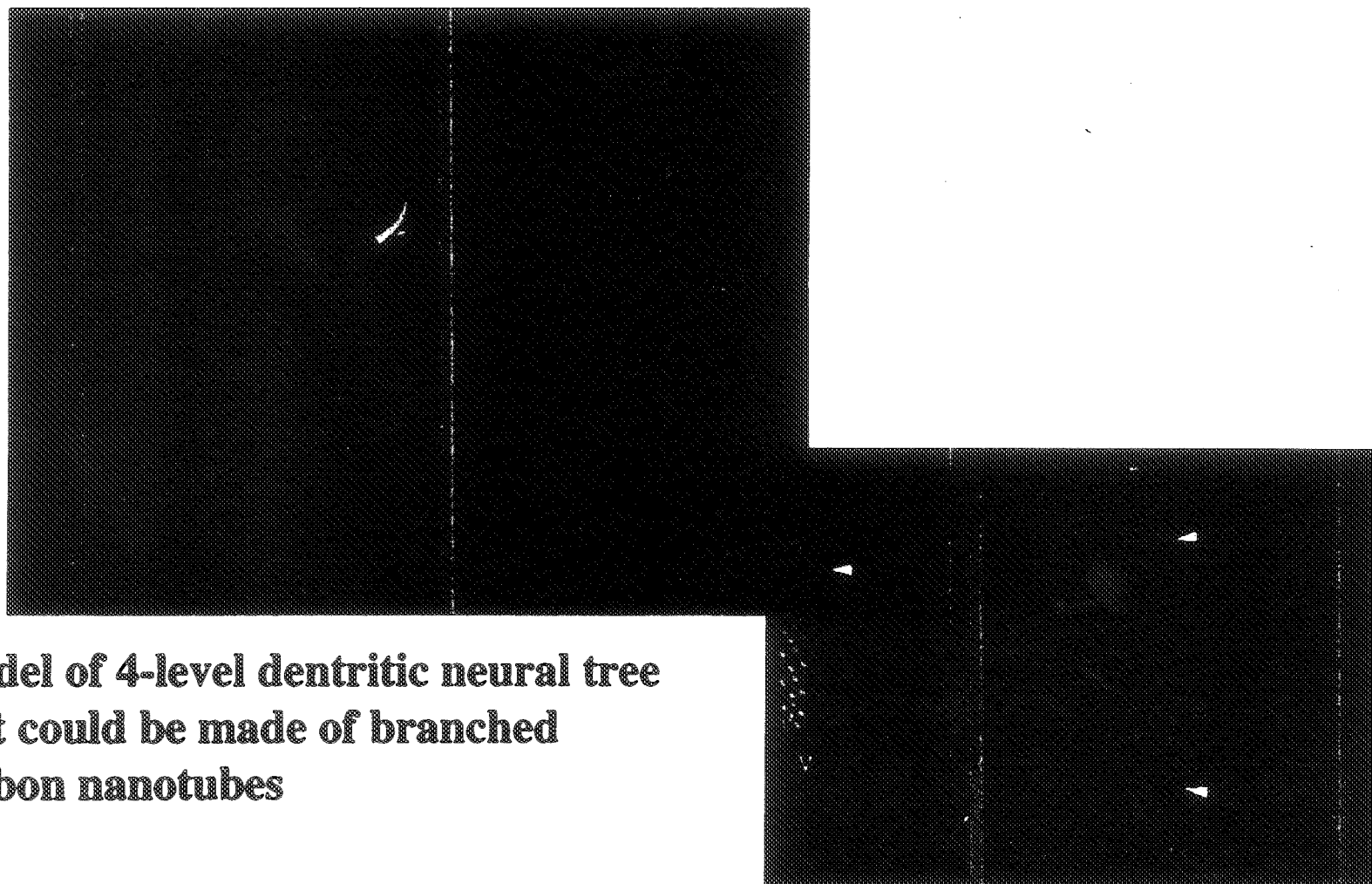
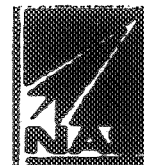
Binding
Energy

D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng And R. Ruoff, J. Phys. Chem. Vol. 103, 4330 (1999).

NASA



**D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng
And R. Ruoff, J. Phys. Chem. Vol. 103, 4330 (1999).**



**Model of 4-level dendritic neural tree
that could be made of branched
carbon nanotubes**

D. Srivastava et. al., Comp. in Science and Engineering, IEEE, APS (2001)