U.S. DEPARTMENT OF ENERGY

Integrated Nanosystems for Atomically Precise Manufacturing

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Workshop
Berkeley, CA
5-6 August 2015

Welcome!

Why are we here?

Definitions

Integrated Nanosystems

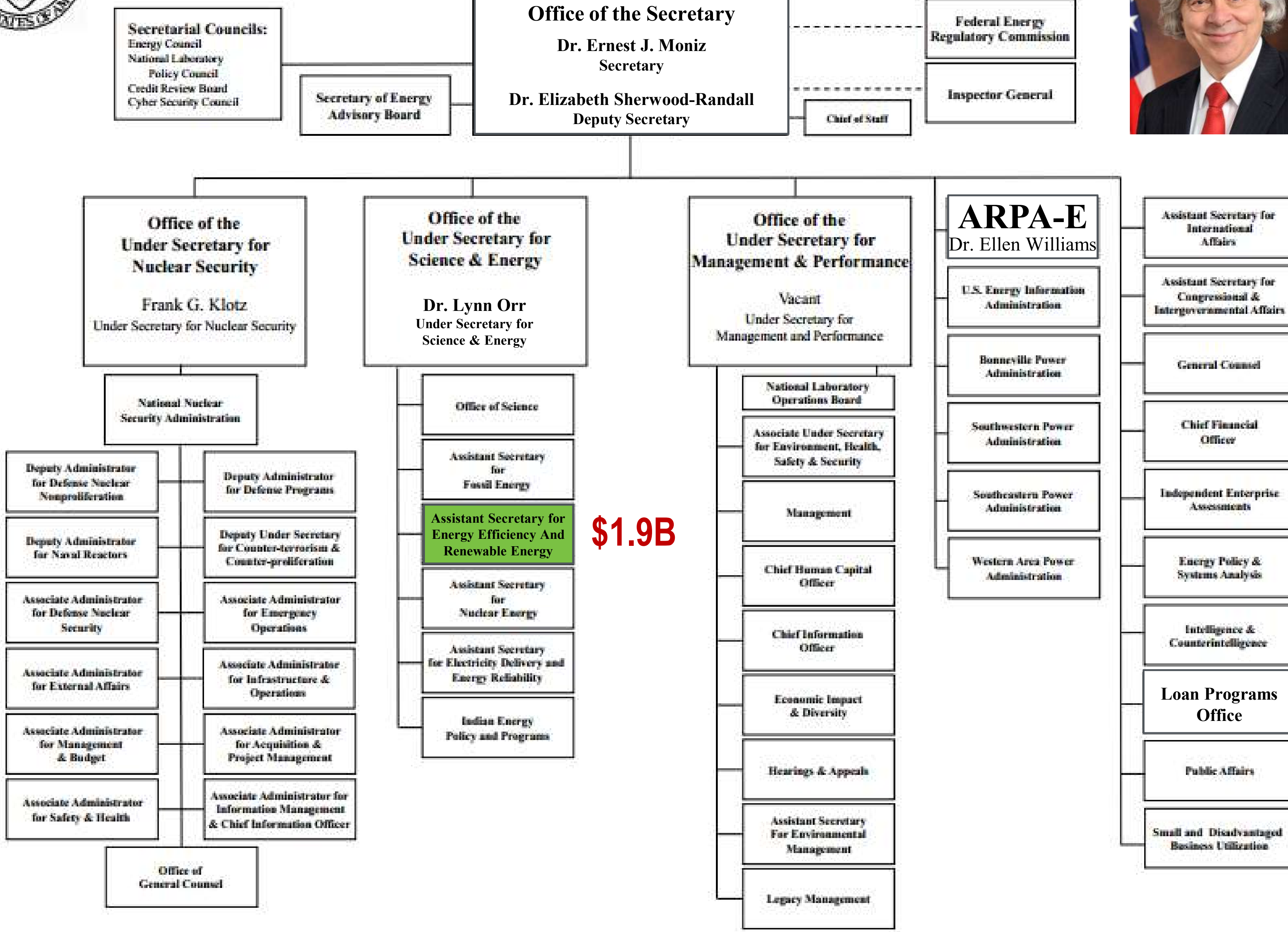
Interconnected mechanical and electromechanical nanoscale devices and nanoscale structural components that operate together to perform a particular task under programmable control

Atomically Precise Manufacturing

Any manufacturing technology that provides the capability to make atomically precise structures, components, and devices under programmable control. *From Productive Nanosystems: A Technology Roadmap (2007)*

DOE Organization Chart

$27B in FY15 **DEPARTMENT OF ENERGY**



EERE Organization Chart

Assistant Secretary
David T. Danielson

Principal Deputy Assistant Secretary
Michael S. Carr

$1.9B

- **Energy Efficiency** – Kathleen B. Hogan
  - **Building Technologies** – Roland J. Risser
  - **Federal Energy Management** – Timothy D. Unruh
  - **Advanced Manufacturing** – Mark A. Johnson ($200M)
  - **Vehicle Technology** – ~~Patrick B. Davis~~
  - **Weatherization & Intergovernmental** – Anna M. Garcia
  - **Sustainability Performance** – Jennifer C. MacDonald
- **Renewable Energy** – Douglas W. Hollett
  - **Biomass Program** – Valerie Sarisky-Reed (*Acting*)
  - **Fuel Cell Technologies** – Sunita Satyapal
  - **Geothermal Technology** – Douglas W. Hollett
  - **Solar Energy Technology** – Minh Sy Le (*Acting*)
  - **Wind & Hydropower Technology** – Jose R. Zayas
- **Business Operations** – Merle L. Sykes
  - **Business Services** – Derek Passarelli (*Acting*)
  - **Budget** – A. Avon Meacham
  - **Information & Business Management** – Douglas E. Kaempf
  - **Project Management & Evaluation** – Scott E. Hine
  - **Golden Field Office** – Carol J. Battershell
- **Strategic Programs** – JoAnn Milliken (*Acting*)
  - **International Program** – Robert L. Sandoli
  - **Analysis & Evaluation** – (*Vacant*)
  - **Communications & Outreach** – Karla Olsen
  - **Innovation & Deployment** – JoAnn Milliken
  - **Legislative, Regulatory & Urban Affairs** – Kerry C. Duggan

Advanced Manufacturing Office (AMO): Purpose

Carbon Fiber from Microwave Assisted Plasma (MAP)

Laser Processing for Additive Manufacturing

AMO's Purpose is to Increase U.S. Manufacturing Competitiveness through:

- ✓ **Manufacturing Efficiency - Broadly Applicable Technologies and Practices**
  - examples: Industrial motors, Combined heat and power (CHP), Industrial efficiency best practices.
- ✓ **Efficiency - Energy Intense Processes**
  - examples: Aluminum, Chemicals, Steel
- ✓ **Cross-cutting Innovations - Clean Energy Manufacturing Technologies**
  - examples: Wide-Bandgap semiconductors, Power electronics, Additive manufacturing, Advanced composites, Roll-to-roll processes, Digital manufacturing

Advanced Manufacturing Office (AMO): Structure

R&D Projects ($84M)

- Manufacturing Efficiency – Broadly Applicable
- Efficiency – for Energy Intense Processes
- Cross-cutting – for Clean Energy Manufacturing Technologies

R&D Facilities ($92.5M)

- Manufacturing Efficiency – Broadly Applicable
- Cross-cutting – for Clean Energy Manufacturing Technologies

Technical Assistance ($23.5M)

- Manufacturing Efficiency – Broadly Applicable

Mandatory Disclaimer

Viewpoints will be treated as informational only, and not as a binding commitment to develop or pursue projects.

Intellectual Property and Openness

Proprietary information is not protected in this forum

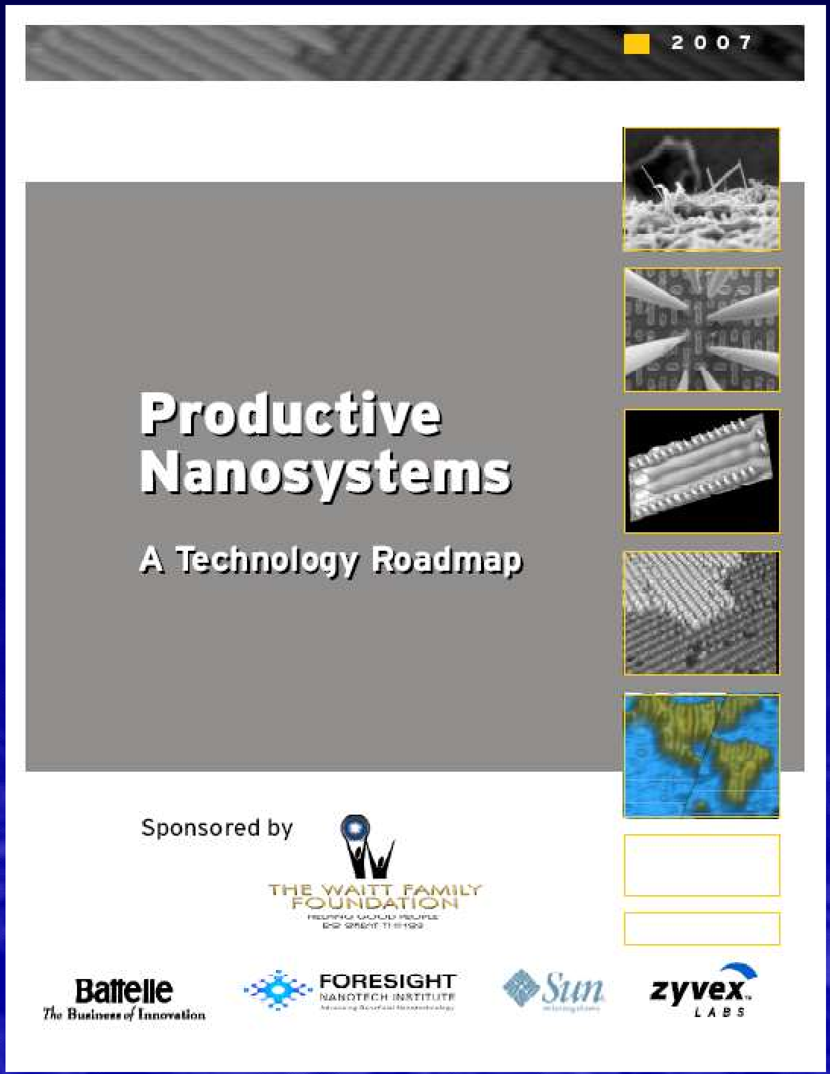
Time	Activity
Wednesday, August 5	
12:00 PM	**REGISTRATION AND BUFFET LUNCH**
1:15 PM	**Welcome and Overview**
1:35 PM	**Keynote Speakers**
2:35 PM	**Core Technologies Presentation**
3:15 PM	**BREAK**
3:30 PM	**Panel Discussion**
4:10 PM	**TRANSITION TO FACILITATED DISCUSSION (Breakout Groups)**
4:15PM	**Facilitated Session I:** Participant Vision and Goals
6:00 PM	**DINNER**
Thursday, August 6	
7:30 AM	**BREAKFAST AND NETWORKING**
8:25 AM	**Welcome and Overview**
8:45 AM	**TRANSITION TO FACILITATED DISCUSSION (Breakout Groups)**
8:50 AM	**Facilitated Session II:** Products and Barriers
10:15 AM	**BREAK**
10:30 AM	**Facilitated Session III:** System Design Pathways and Scale-up; Foundational and Applied R&D Needs?
12:00 PM	**LUNCH**
1:00 PM	**Facilitated Session IV:** Verification, Characterization, and Demonstration
2:15 PM	**Large Group Discussion**
3:00 PM	**Closing Remarks**
3:15 PM	**ADJOURN**

Motivation

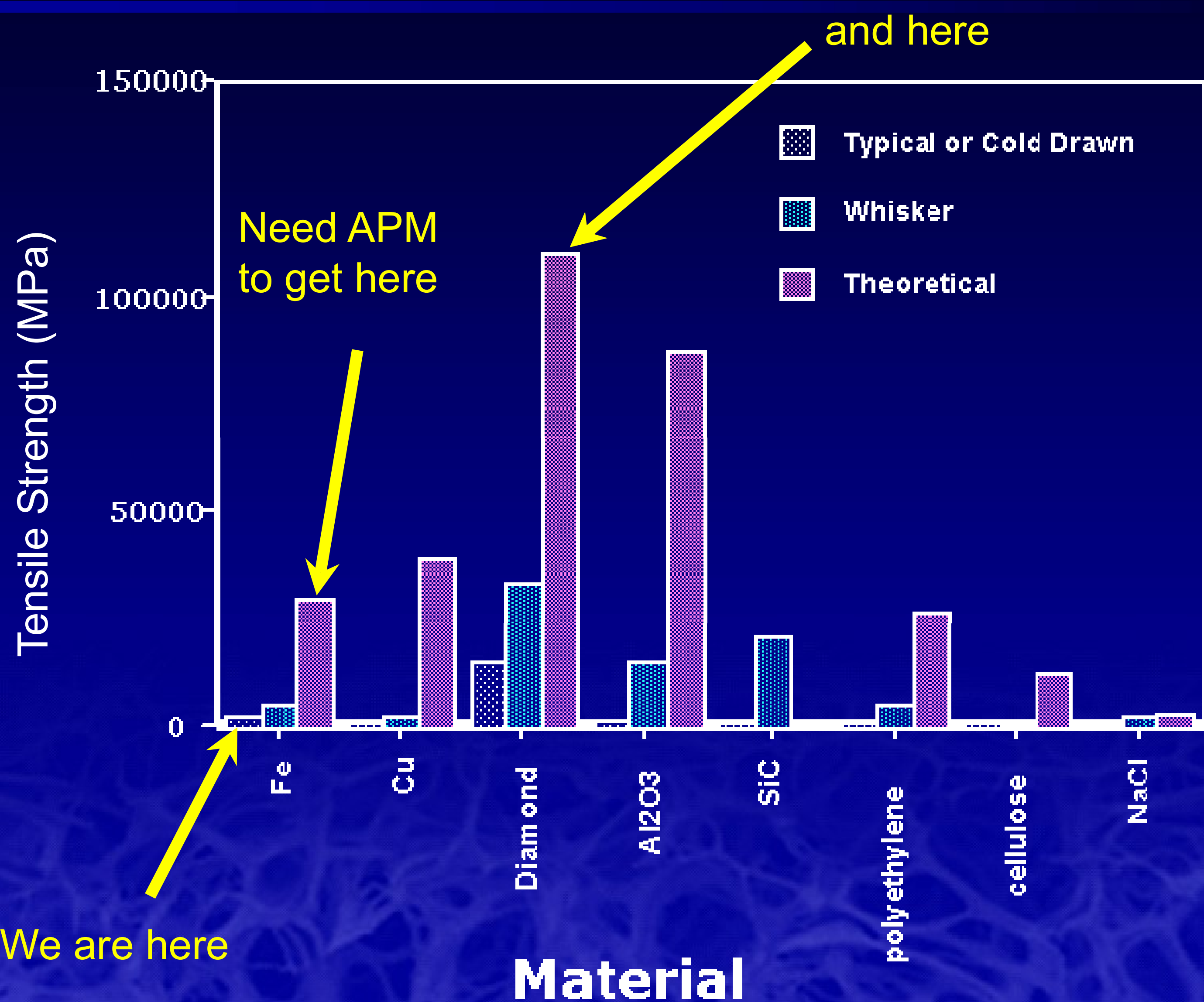
- Atomically Precise Manufacturing
- Integrated Nanosystems

Motivation

- Atomically Precise Manufacturing
- Integrated Nanosystems

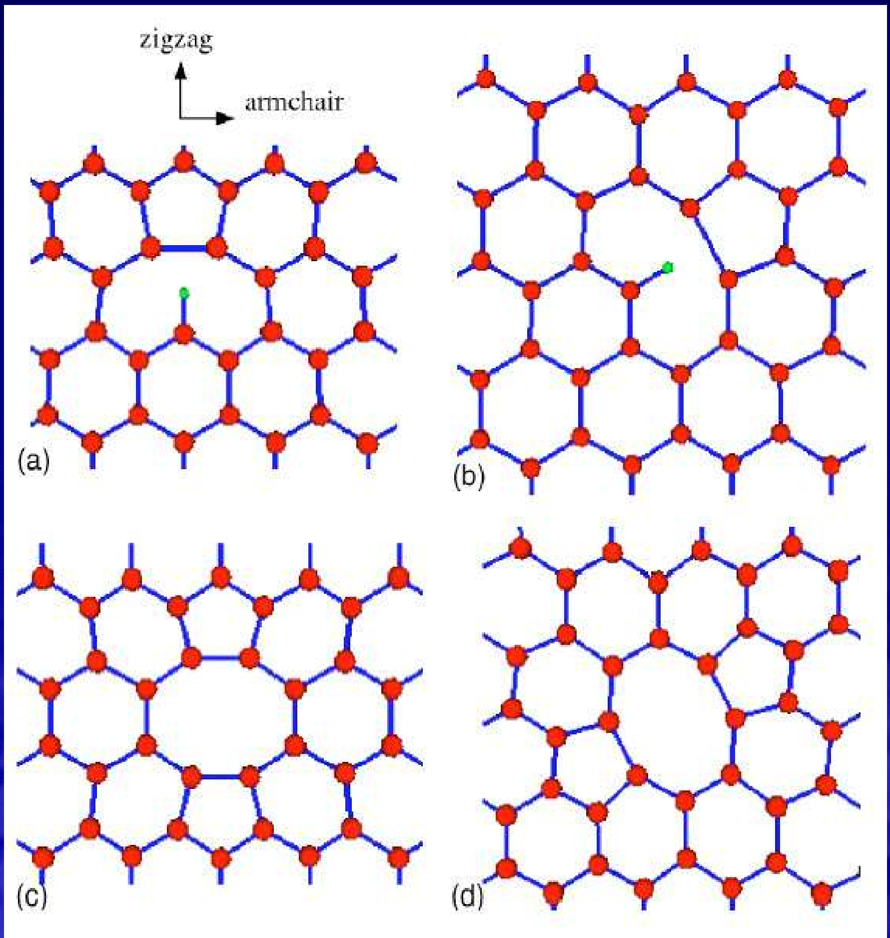


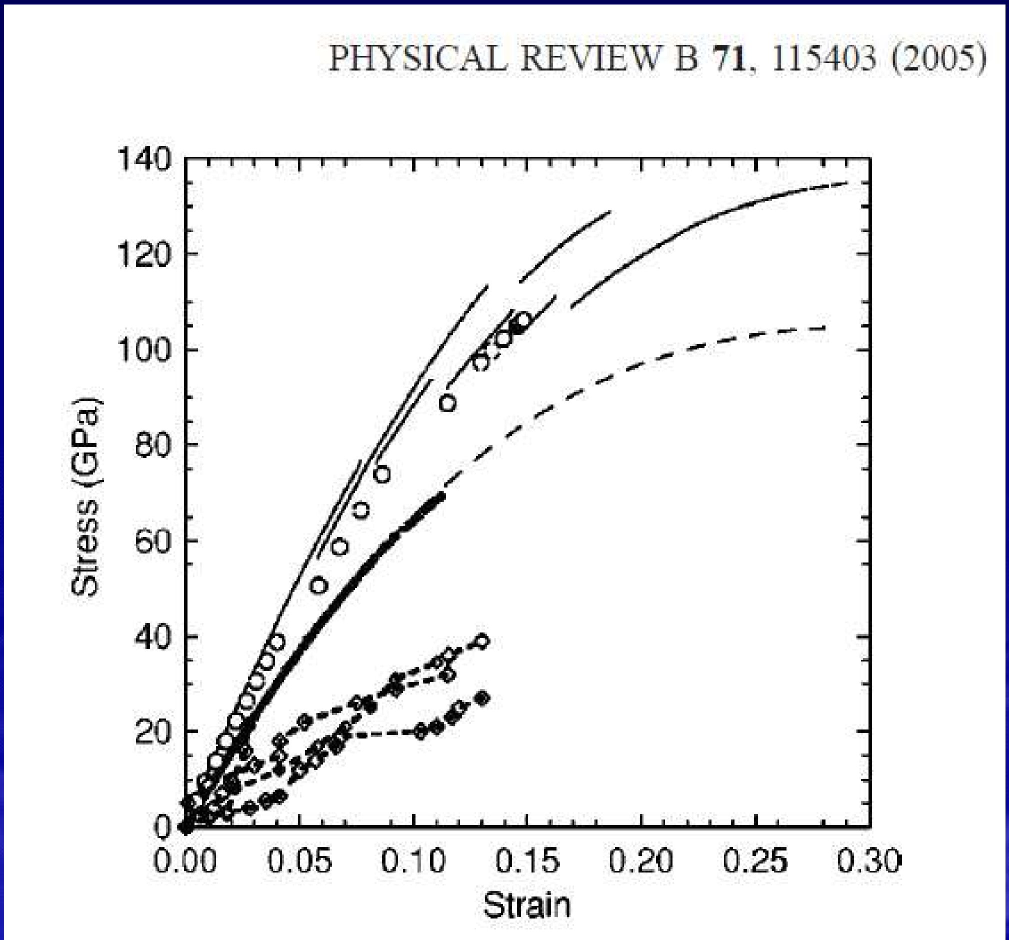
Strength Bandwidth



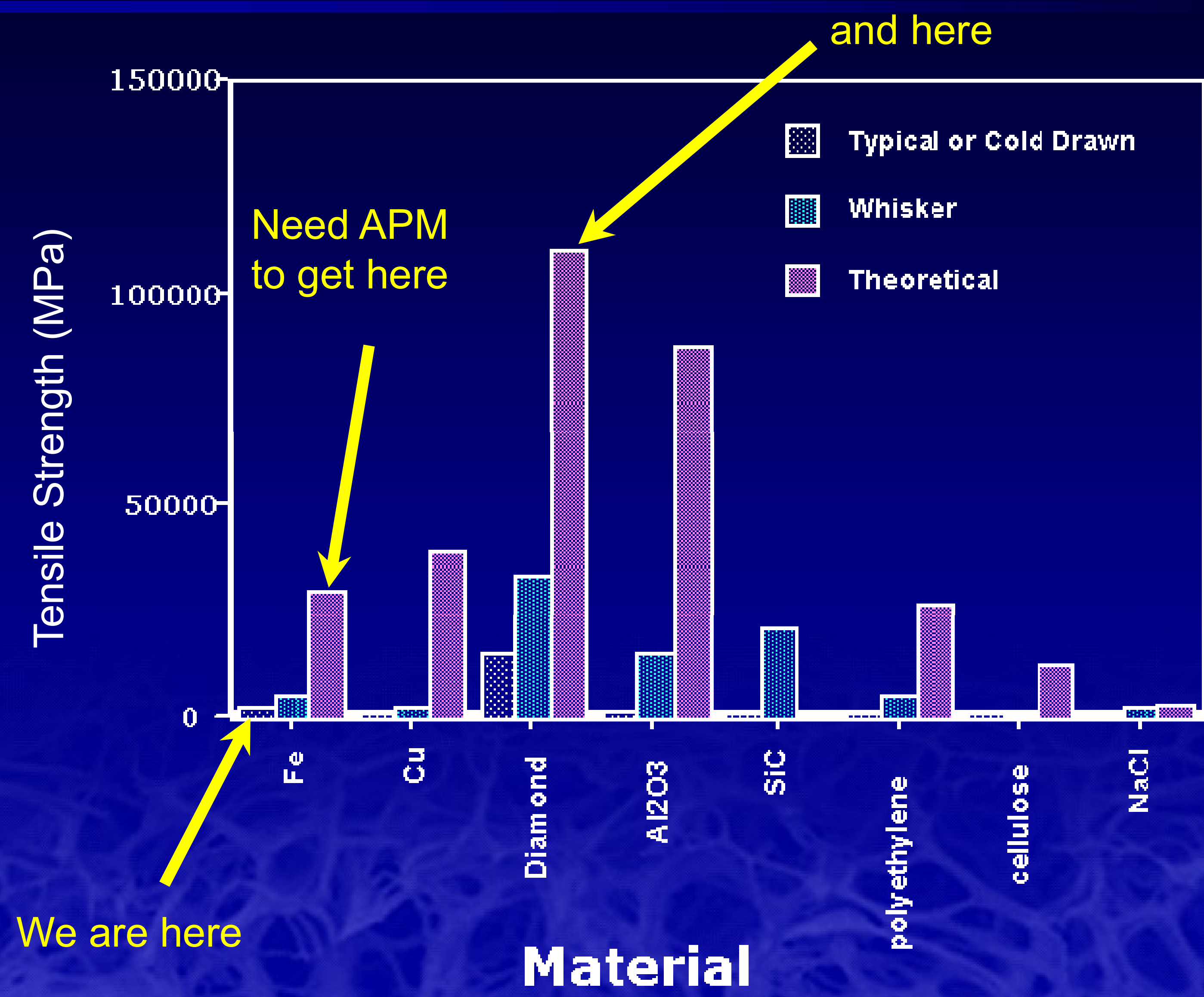
Nanotube Lattice Defects

- Defects reduce strength of C nanotubes



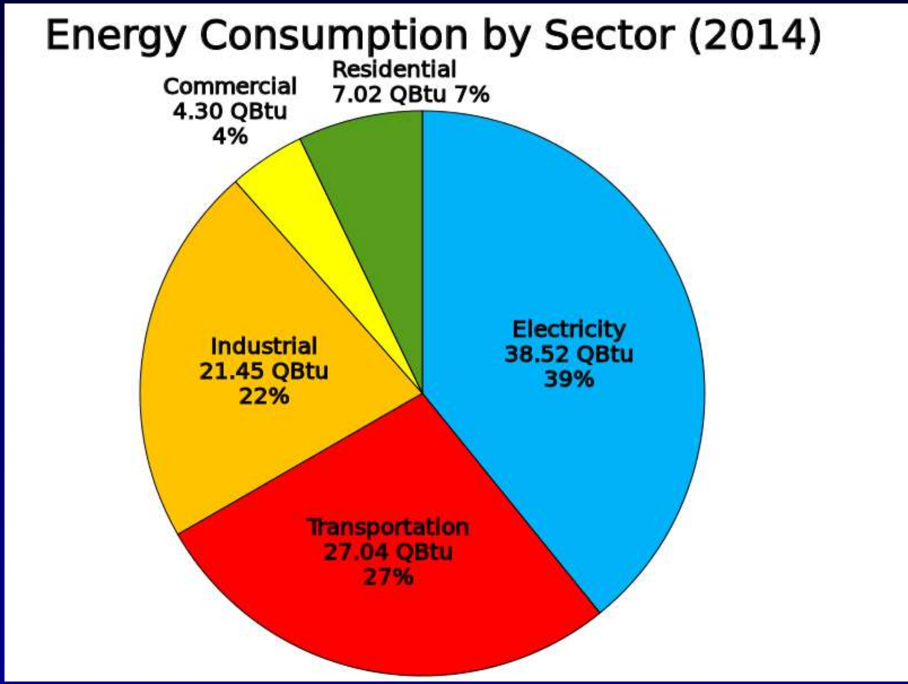


Strength Bandwidth



Reduction in Energy Consumption

- Lightweighting
  (90% weight reductions)
- Transportation:
  27 Quads down to 3 Quads
- Industrial processes
  (90% reduction in amount of material produced);
  21 Quads down to 2



- Improved efficiencies in electricity generation
- Penalty for bandwidth gap: 50 Quads annually

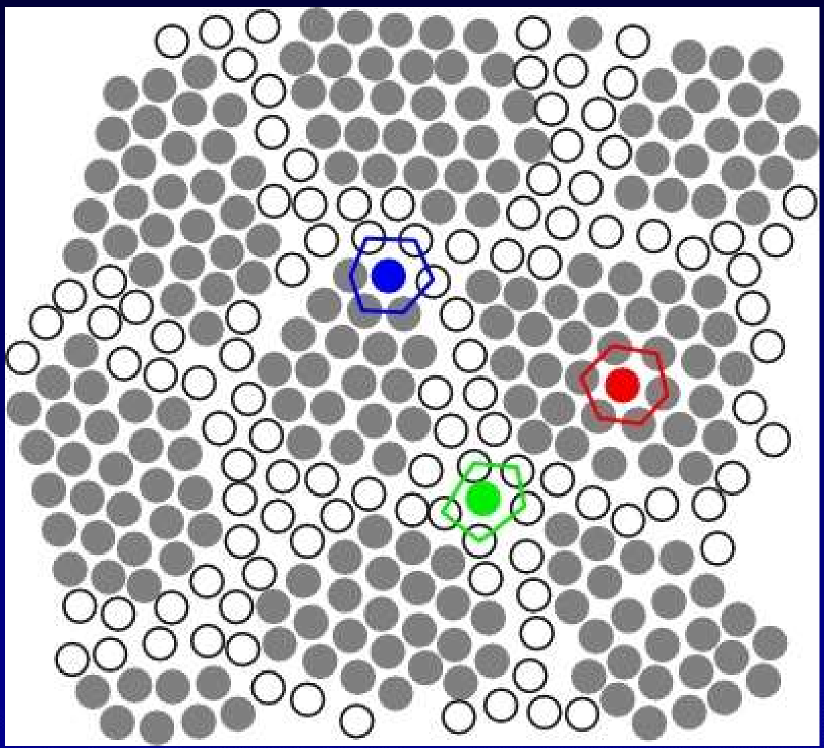
To Do List

1) Detailed analysis to verify 50 Quads annual energy savings with APM

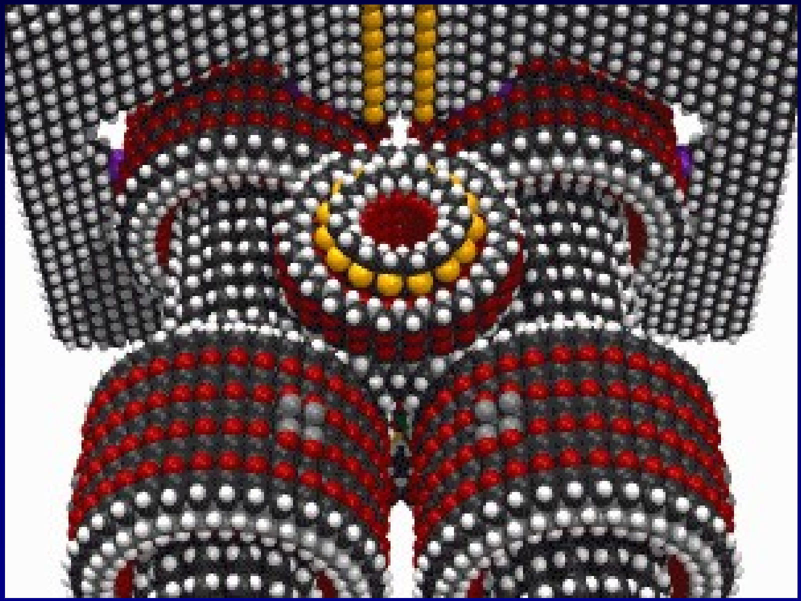
On Defects

- Have been told that the material would "explode" if you tried to make it defect free
- Have been told that we already make atomically perfect material (silicon single crystal)
- Have been told that we already have atomically precise manufacturing (atomic layer deposition)
- Have been told that materials design with perfect single crystals is problematic from both plastic and elastic stretching standpoints

All nanosystems are not created equal



In polycrystalline materials, grains are surrounded by disordered boundaries, promoting defect structures that equilibrate at high temperature



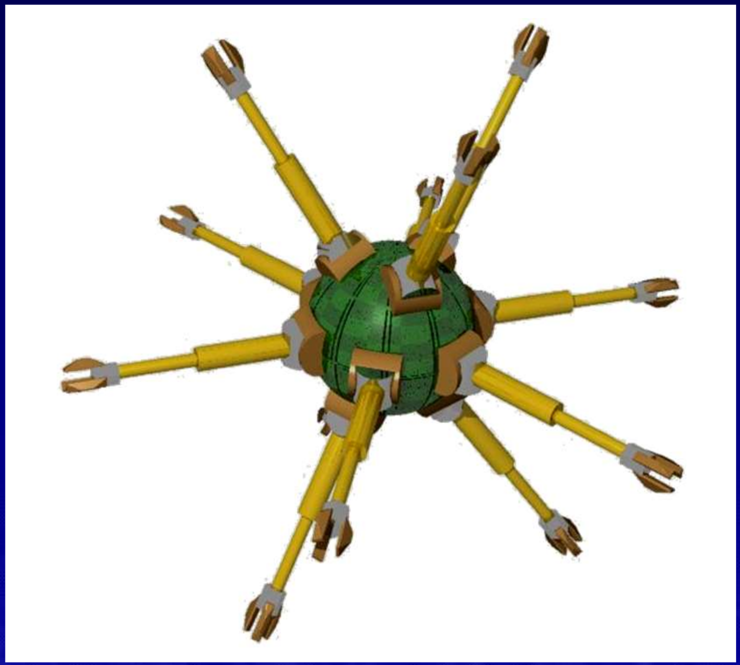
Molecular Worm Drive with atomically precise surfaces that are well-terminated , synthesized at low temperature, is less likely to form spontaneous defects (Nanorex)

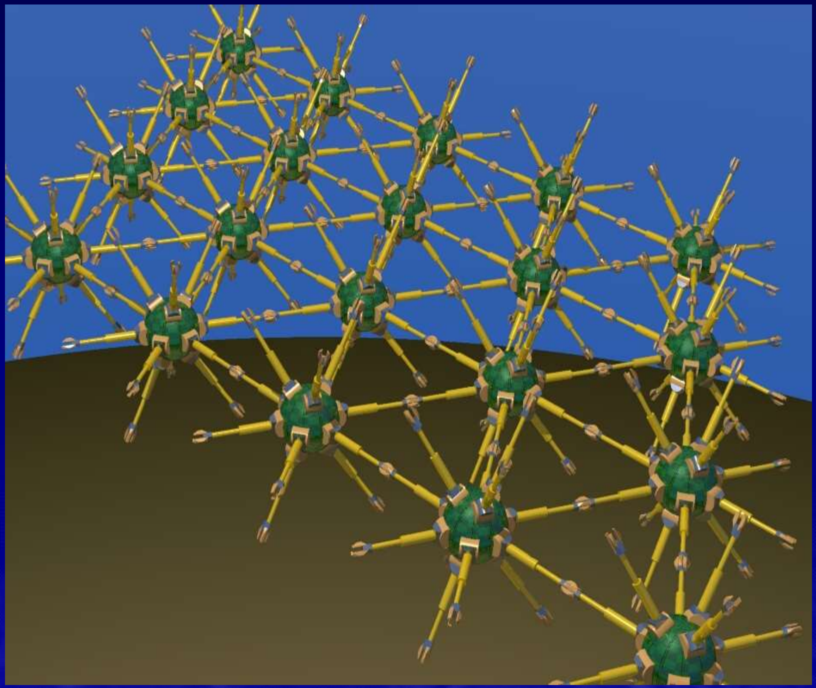
To Do List

1) Detailed analysis to verify 50 Quads annual energy savings with APM
2) Fundamental science studies are needed to understand defect formation in macroscopic atomically precise materials and devices

Dynamic Strain Accommodation

Rich integration of computers, sensors, and actuators → programmable materials





- Telescoping arms and nanoscale actuators could compensate for high (10%) elastic strains needed for strength
- Telescoping arms could accommodate large deformations and internal systems could reversibly store/dissipate energy

To Do List

1) Detailed analysis to verify 50 Quads annual energy savings with APM
2) Fundamental science studies are needed to understand defect formation in macroscopic atomically precise materials and devices
3) Need detailed system designs and analysis of deformable space frame materials

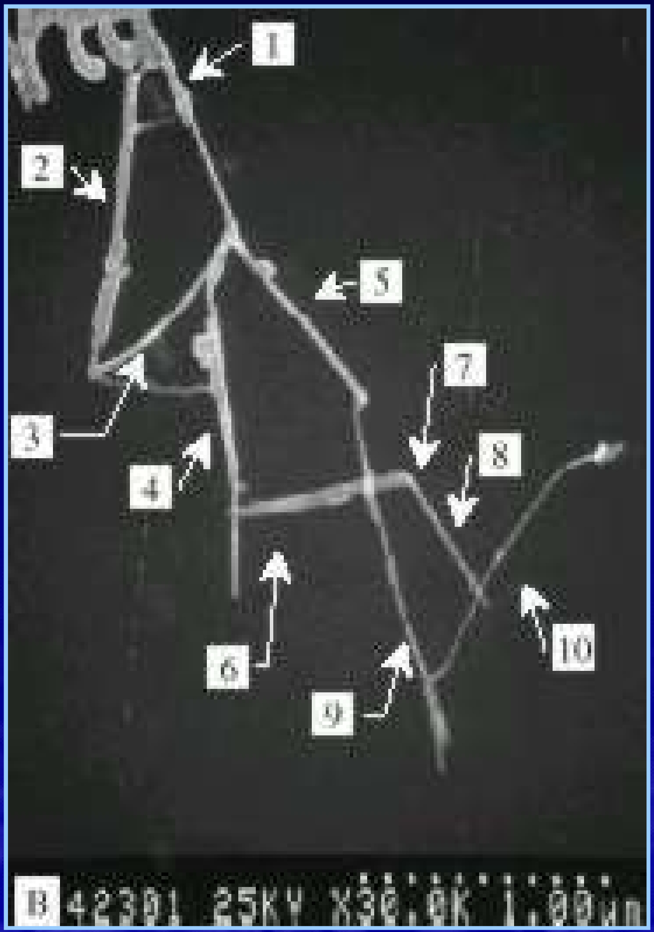
Why Integrated Nanosystems?

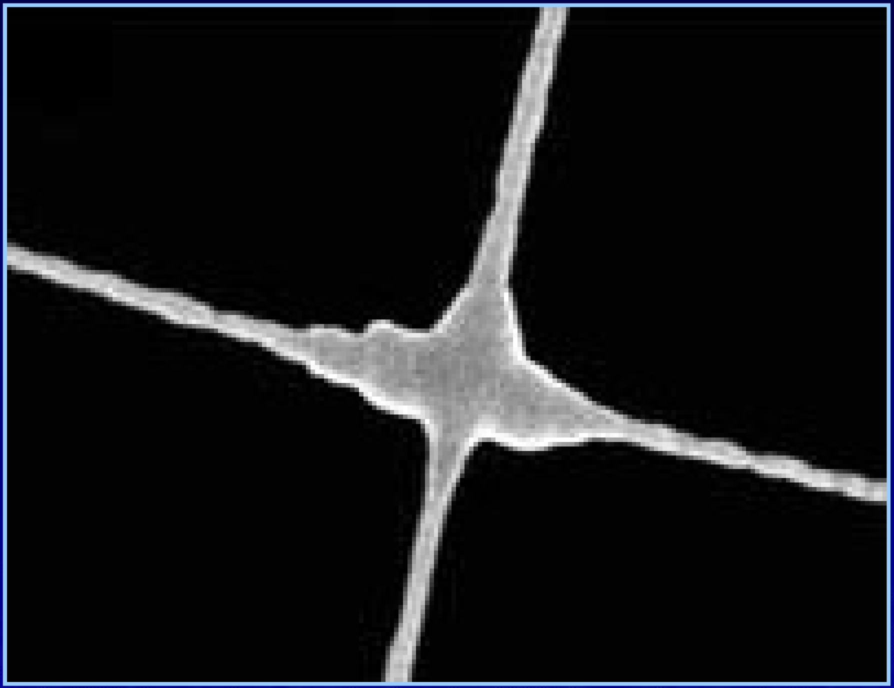
- Condensing matter from solution, vapor, or melt fundamentally <u>cannot</u> produce atomically precise structures.
- Left with self-assembly of atomically precise building blocks, or with positional assembly
- Compelling vision for a scalable high throughput system based on positional assembly presented by Drexler (Nanosystems (1991) and elsewhere)
- Recent advances point to a potential approach

Nanotube Welding

Skidmore, et al., 1999

http://people.nas.nasa.gov/~globus/papers/NanoSpace1999/paper.html

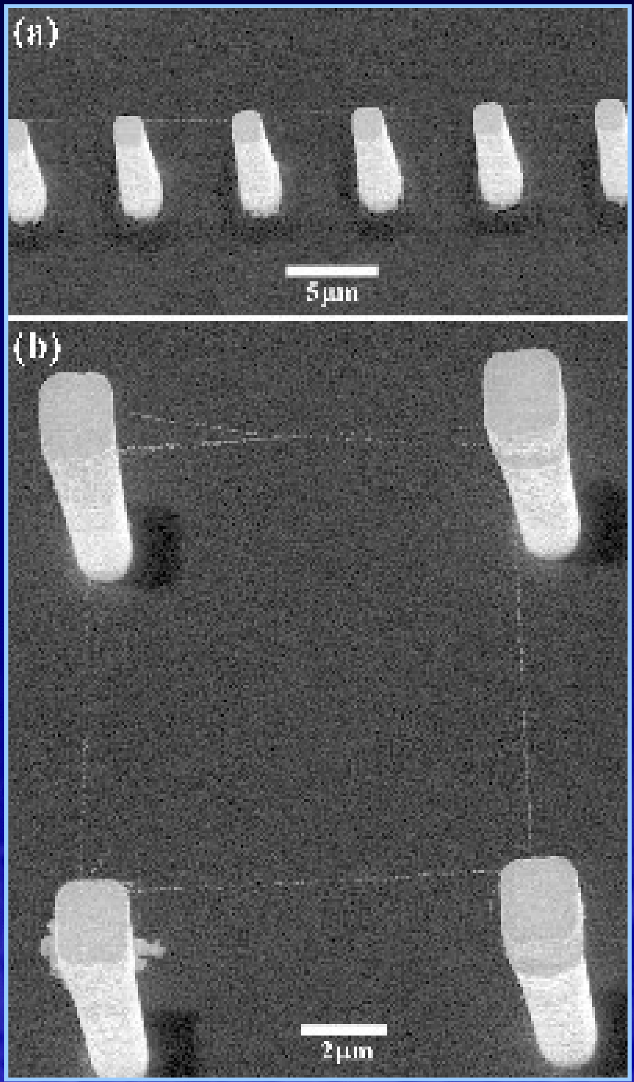




Florian Banhart, "The formation of a connection between carbon nanotubes in an electron beam," Nano Letters 1, 329-332 (2001).

Nanotube Suspension

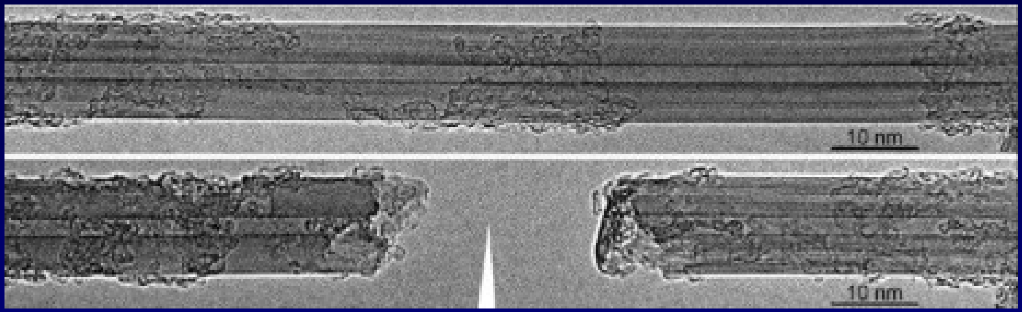
(Cassell, et al., 1999)



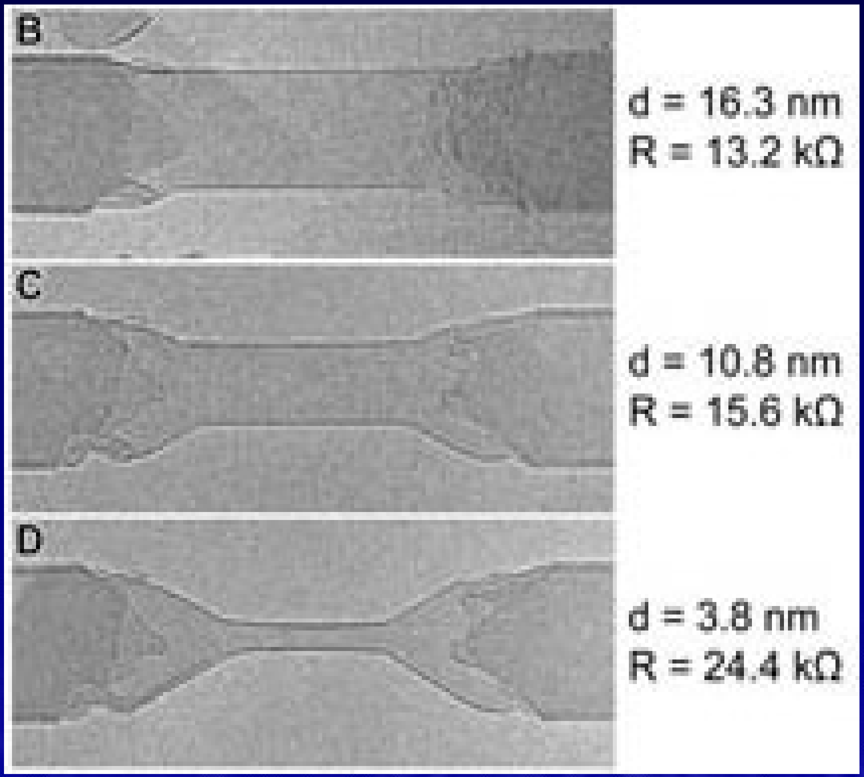
Skidmore, et al., 1999

Nanotube construction

(Zettl)

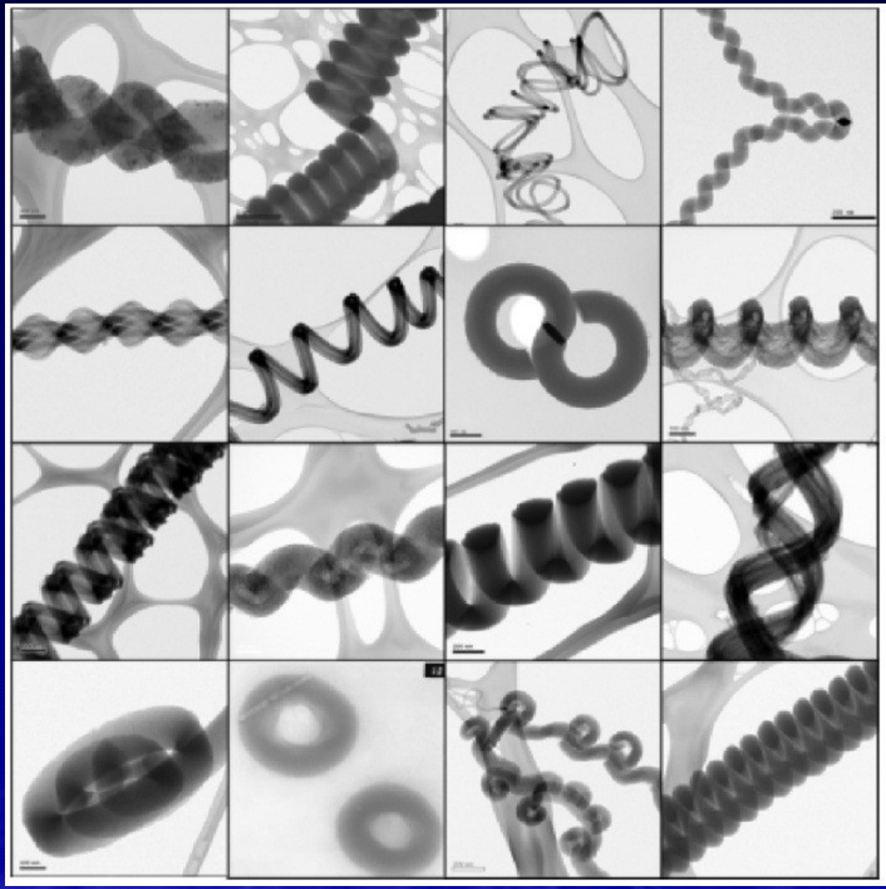


Cut to length



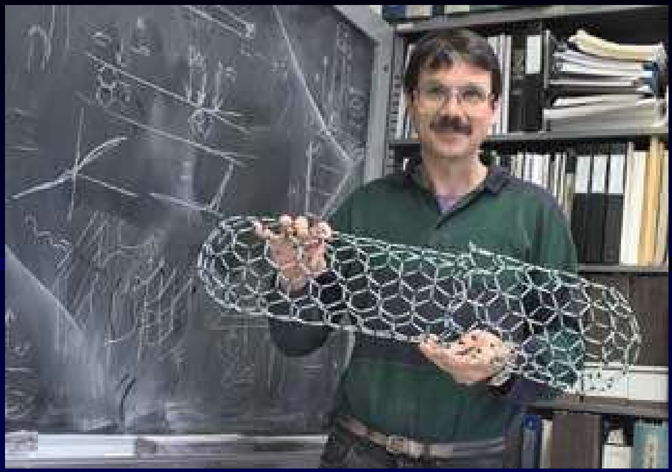
Ablate outer walls

Nanosprings



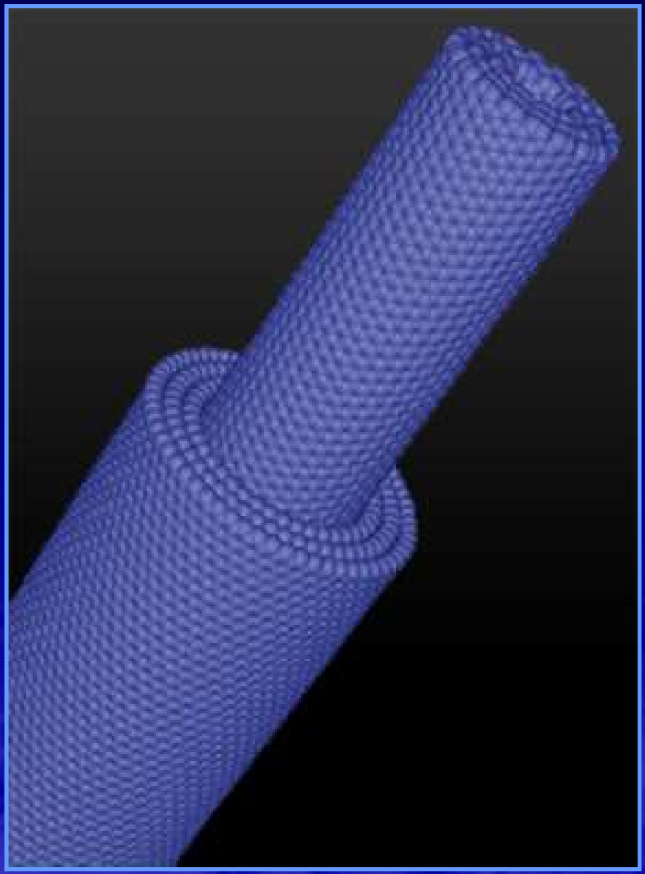
Nanotechnology and Nanomaterials » "Syntheses and Applications of Carbon Nanotubes and Their Composites", book edited by Satoru Suzuki , ISBN 978-953-51-1125-2, Published: May 9, 2013 under CC BY 3.0 license. © The Author(s).

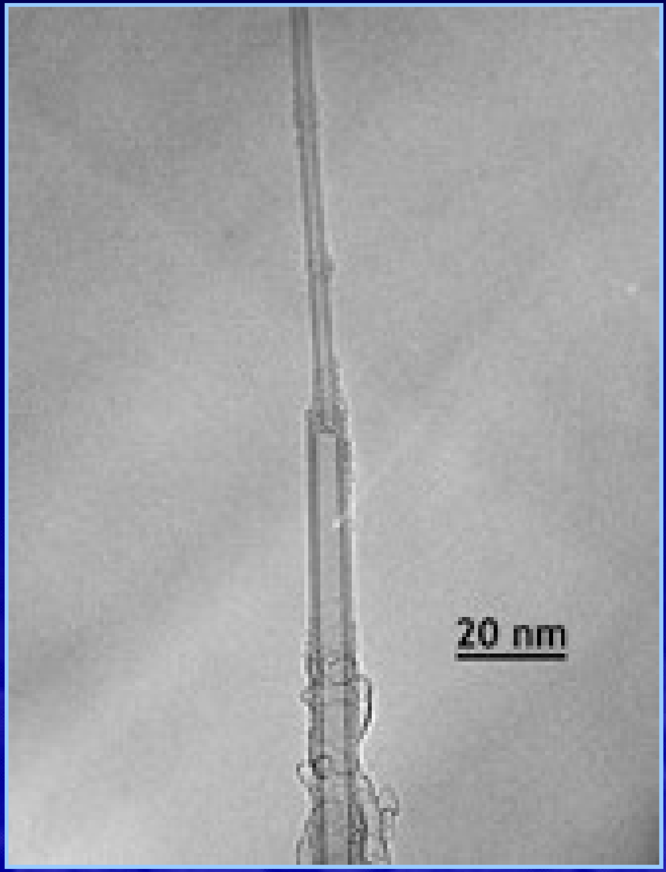
Telescoping Nanotubes



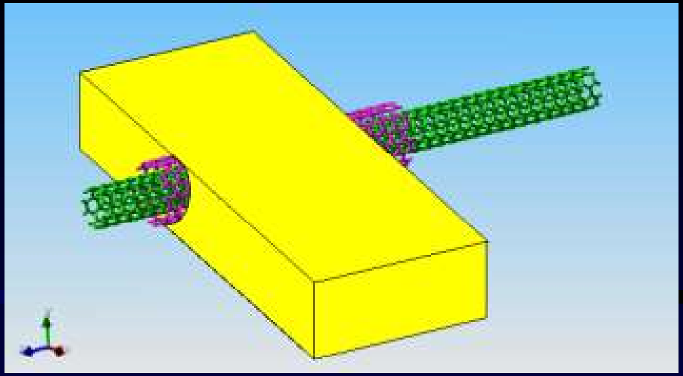
(Zettl, Lawrence Berkeley Laboratory, 2001)

http://www.lbl.gov/Science-Articles/Research-Review/Magazine/2001/Fall/features/02Nanotubes.html

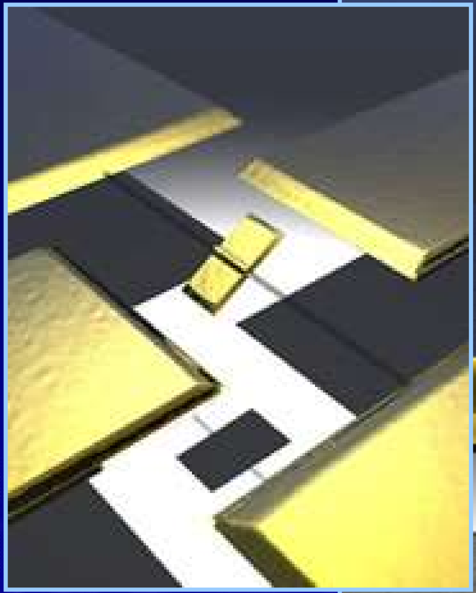


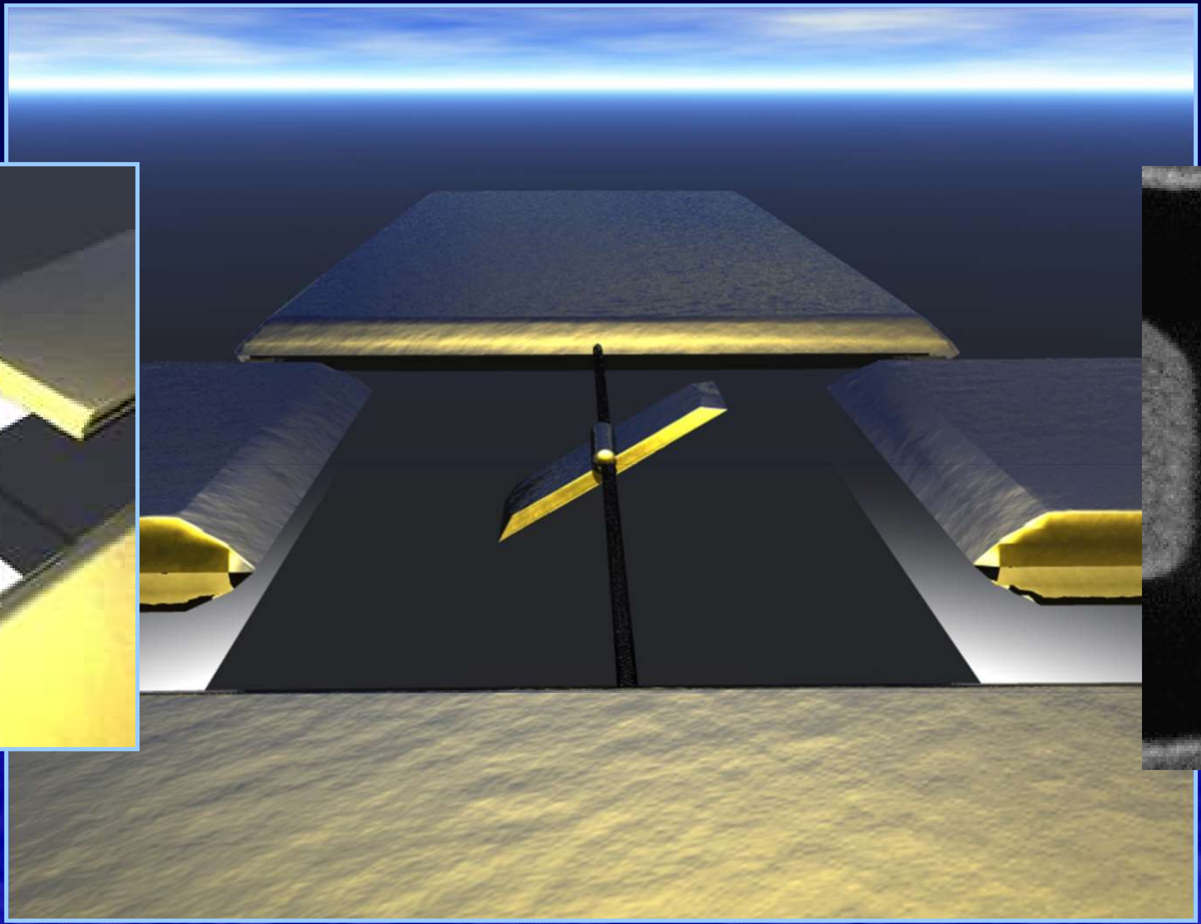


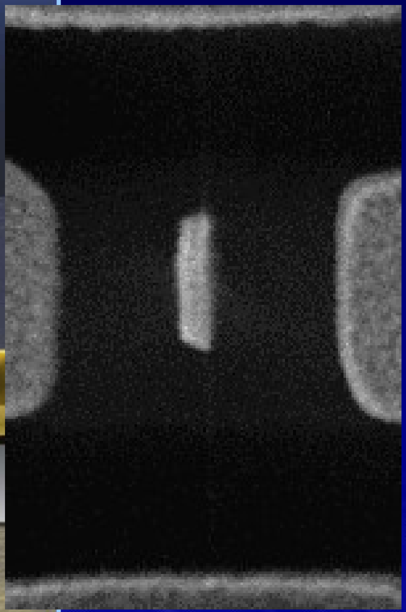
Molecular Motor



(Zettl, LLNL and U.C. Berkeley, 2003)

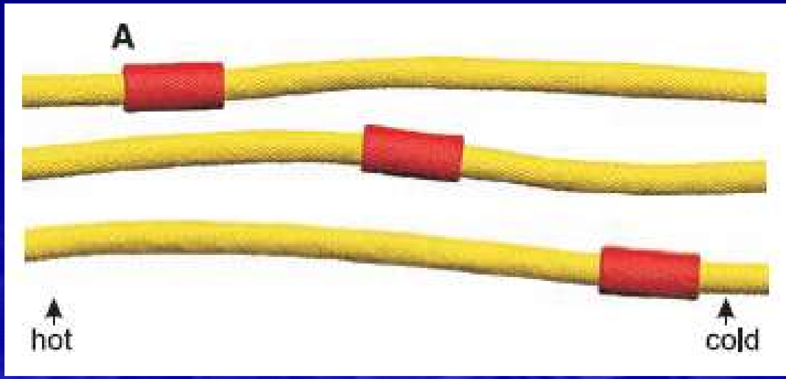


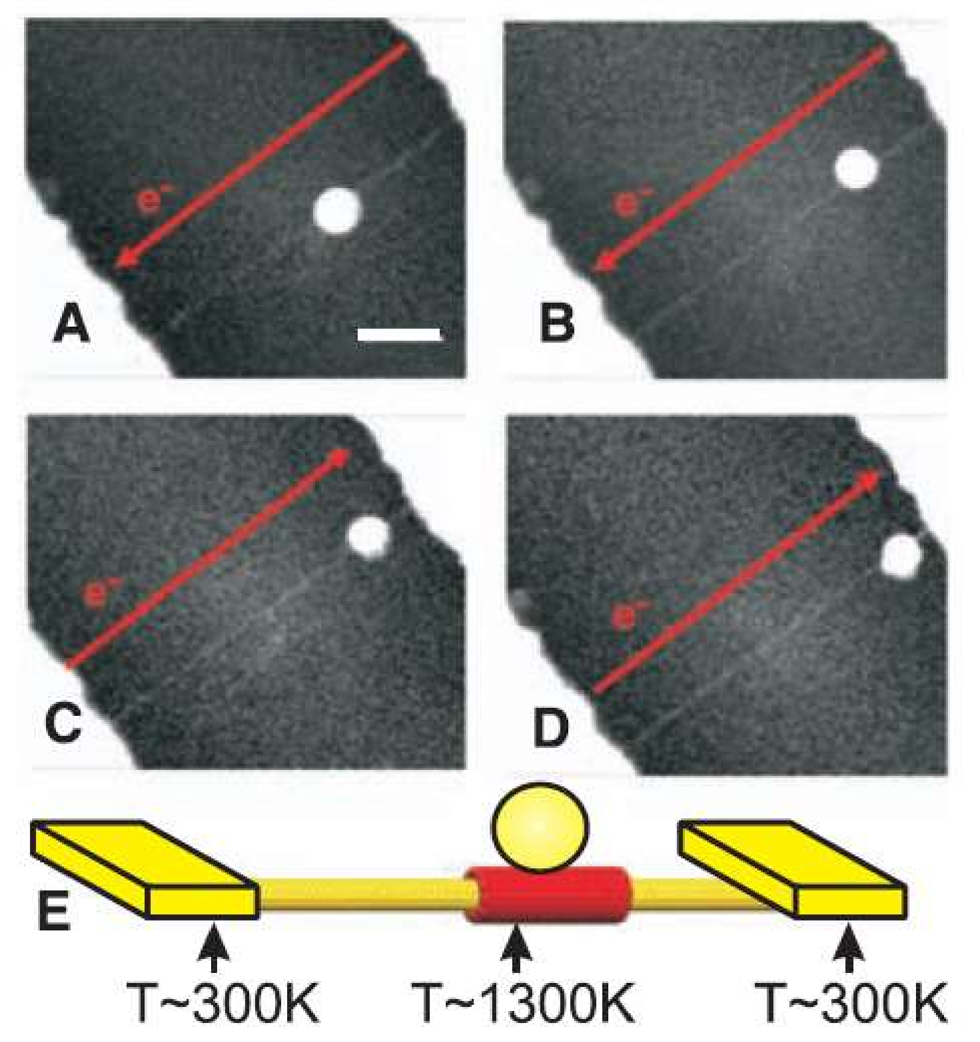




Linear actuation of nanomechanical devices

- Driven by thermal gradient caused by electrical resistive heating
- Gold sphere as marker
- Gradient: a few K/nm
- Speed: ~ 1 μm/s

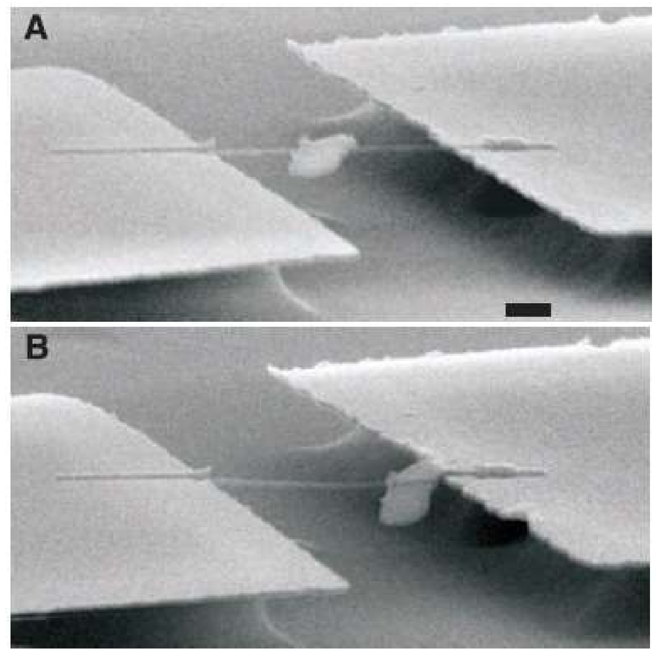




Barreiro, et al., "Subnanometer Motion of Cargoes Driven by Thermal Gradients Along Carbon Nanotubes," *Science*, v. 320, 9 May 2008, 775-778.

Linear actuation of nanomechanical devices

- Driven by thermal gradient caused by electrical resistive heating (0.1 mA)
- Rotational motion as well



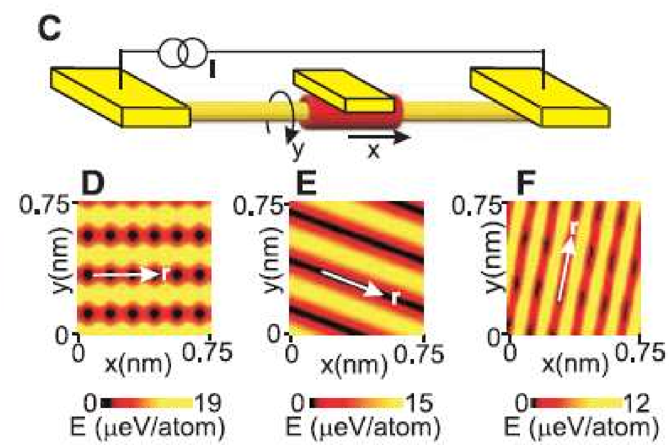
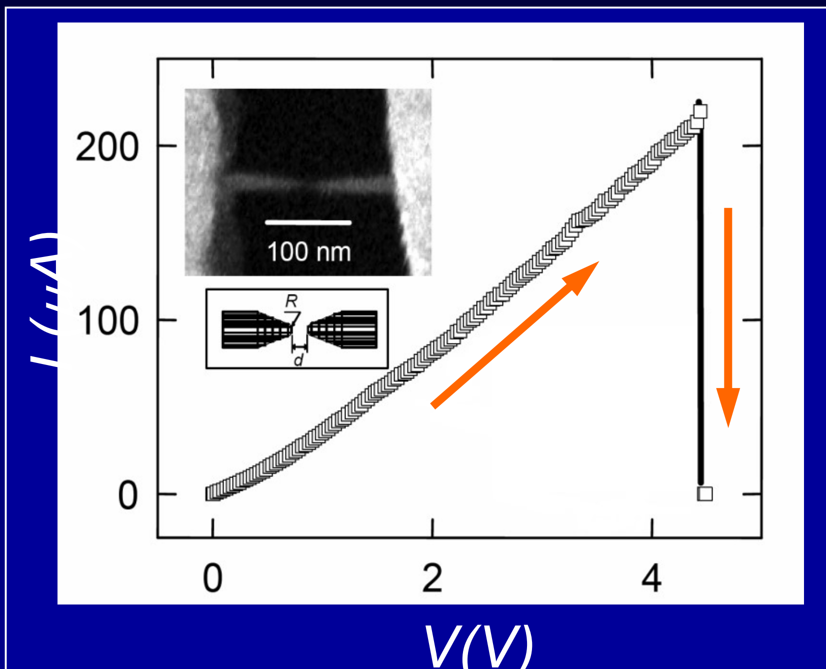


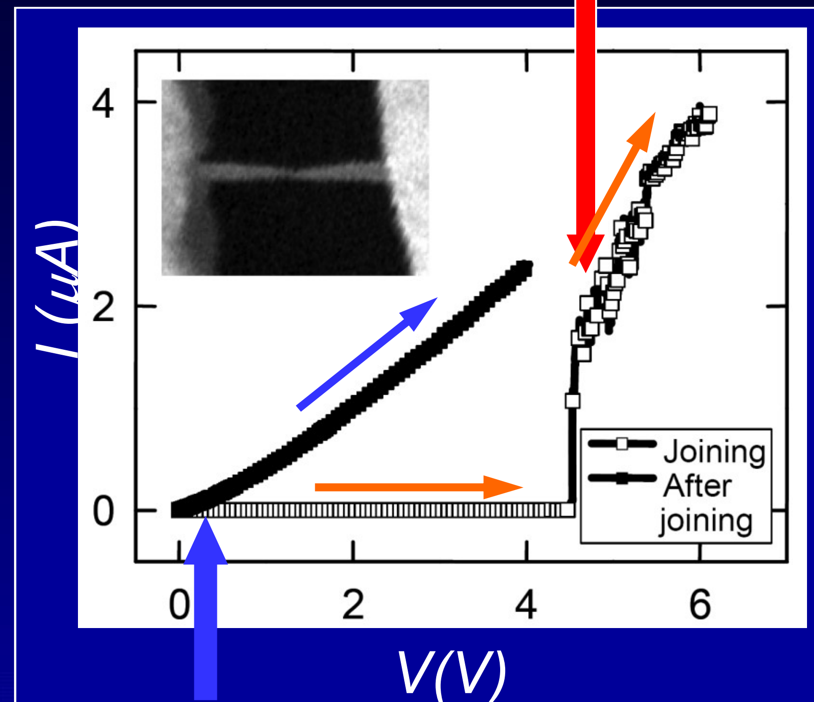
Fig. 1. Experimental setup. (**A** and **B**) Scanning electron microscope (SEM) images of one device where the central object attached to nanotube in (A) has been moved via an AFM tip. Scale bar in (A), 300 nm. (**C**) Schematic of the nanotube motor and its degrees of freedom. The outer (red) nanotube moves with respect to the inner (yellow) nanotube. *I*, the current. (**D** to **F**) Shape of the energy barrier for the relative motion between two coaxial nanotubes: (5,5)/(10,10), (29,9)/(38,8), and (27,12)/(32,17), respectively. The diameters of the inner tubes are 0.67, 2.7, and 2.7 nm, respectively. The white arrows indicate the easy axis of motion (*r*). The motion is modulated by a series of small periodic barriers in (D) and (F), whereas vanishingly small friction is expected in (E).

Barreiro, et al., "Subnanometer Motion of Cargoes Driven by Thermal Gradients Along Carbon Nanotubes," *Science*, v. 320, 9 May 2008, 775-778.

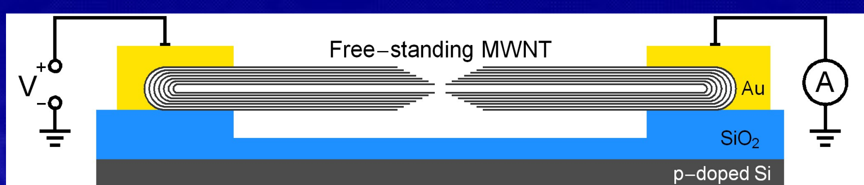
Linear actuation of nanomechanical devices

inner shells extend and close gap





Tube ends adhere, latching conductive state (ON state)

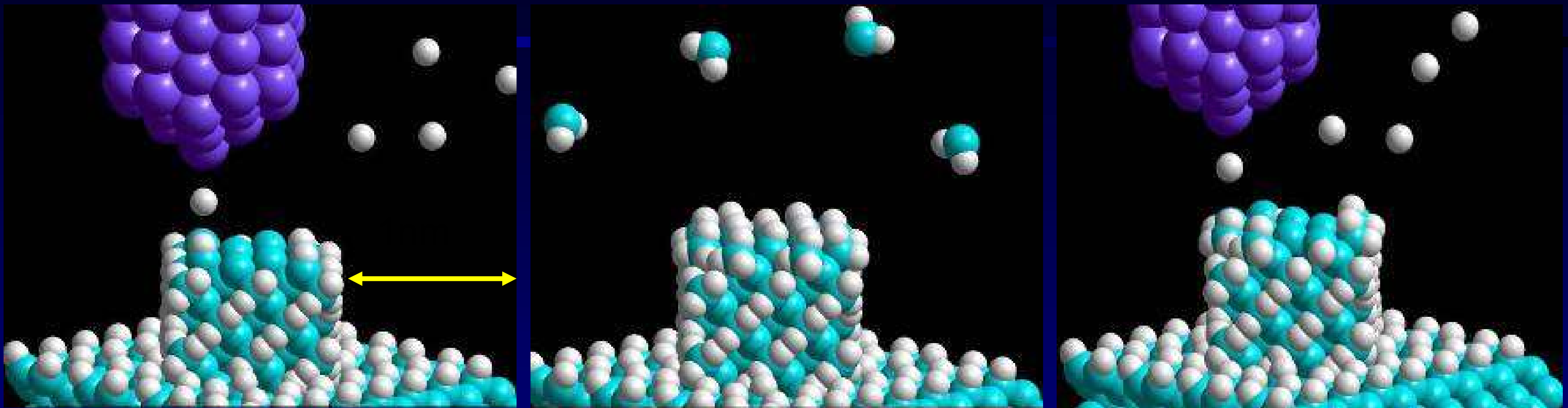


MWNT linear bearing nanoswitch
Creating the initial OFF state

Marc Bockrath
UC Riverside

Deshpande,, et al., "Carbon Nanotube Linear Bearing Nanoswitches," *Science*, v. 320, 9 May 2008, 775-778.

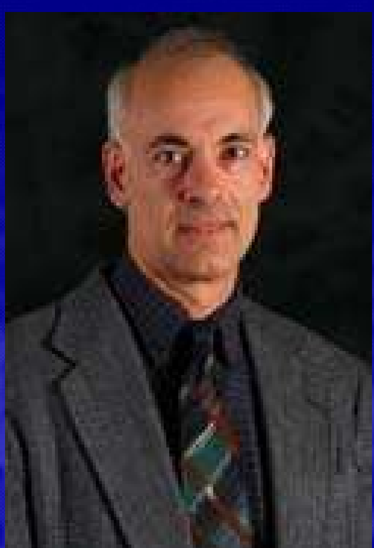
Additive Manufacturing at the Atomic Level



Invariant atomically-precise STM tip, with closed loop computer control, inside UHV system, removes H from Si surface with atomic precision

In deposition phase, gaseous SiH_2 radicals deposit one Si atom wherever H atom is removed (patterned Atomic Layer Epitaxy)

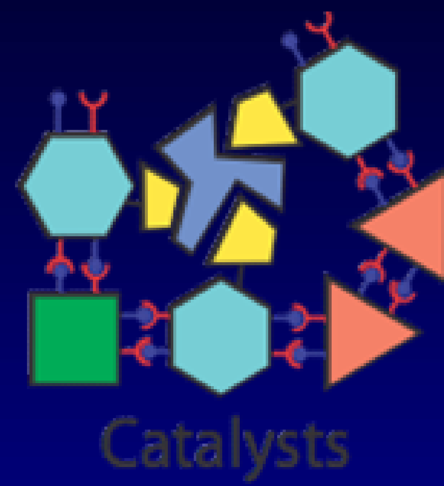
After each deposition cycle, SiH_2 is evacuated and patterning step is repeated to create designed 3D structure

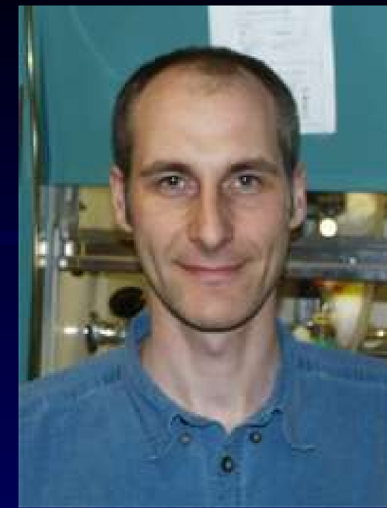


- APM is the integration of two known experimental techniques:
  - The atomic precision removal of H atoms from a silicon surface
  - Atomic Layer epitaxy: the deposition of a single layer of Si atoms
- The process is repeated to build up 3D structures.
- The process could make both near term applications and <u>can be scaled</u> to make a wide variety of future applications

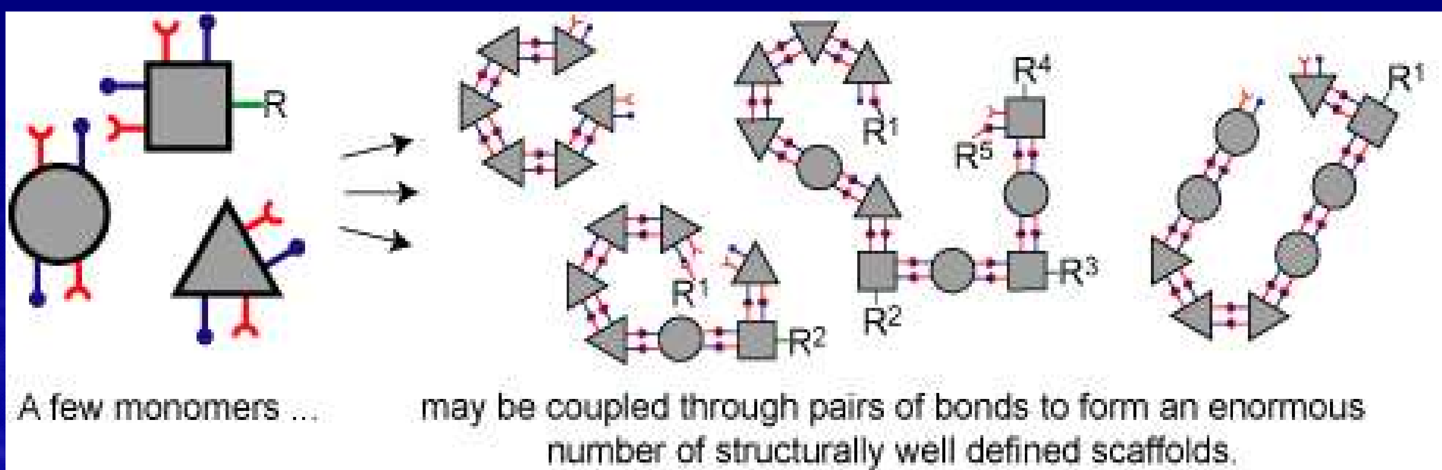
Prof. Joe Lyding: Beckman Institute, Urbana, IL

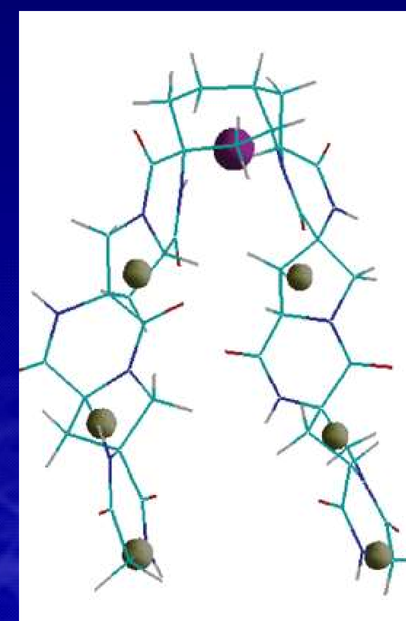
Molecular Lego®





Chris Schafmeister
Temple University



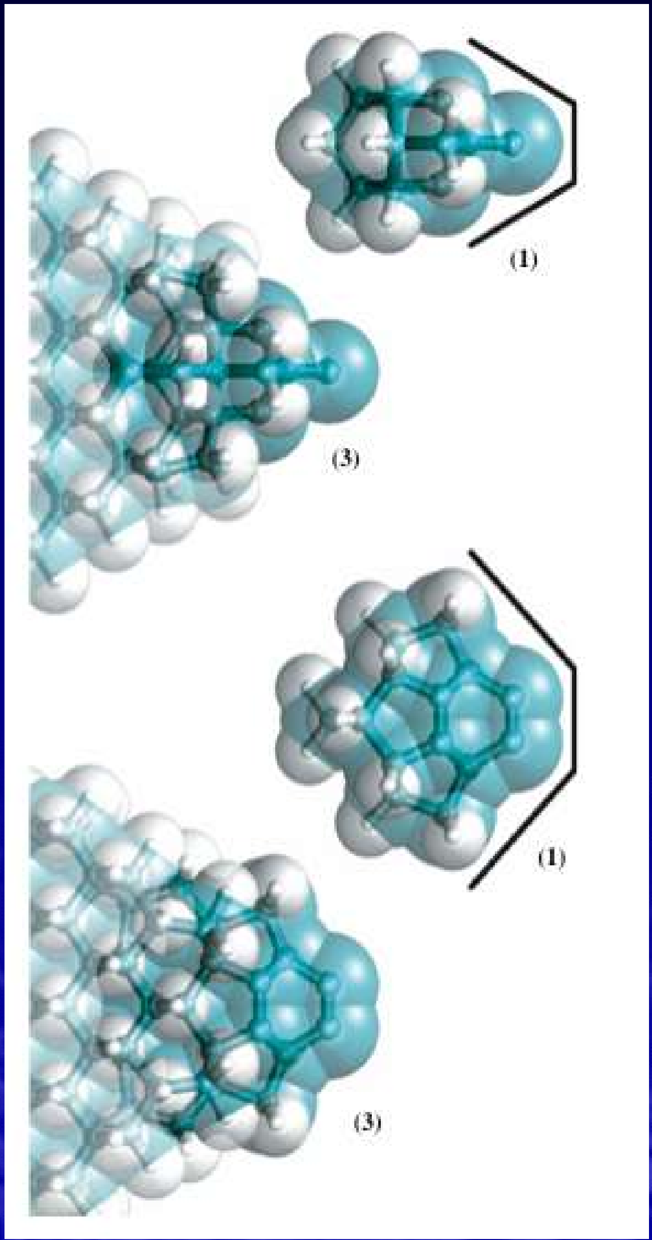


http://www.temple.edu/chemistry/directory/faculty/schafmeister/

Theory: Diamondoid Mechanosynthesis

Allis, D.G. and K.E. Drexler (2005) Design and Analysis of a Molecular Tool for Carbon Transfer in Mechanosynthesis, *J. Comput. Theor. Nanosci* **2:**45-55

- Tool for building diamondoid structures
- DFT-based analysis, 6-31G(d,p) Gaussian-type basis set25 and B3LYP density functional
- Extensive treatment of reliability and failure modes



Animation

- transport individual feedstock molecules to the workspace (actively or passively)
- modify the feedstock (if required) to prepare it for the assembly operation
- manipulate or transport the feedstock to the attachment point at a specified atomic position
- chemically bind the feedstock to a growing structure or device at that attachment point
- repeat the operation a sufficient number of times to synthesize a product with no defects

Why a demonstration nanosystem?

- Focus attention on an important technology space
- De-risk the concept for funding agencies
- Decisive step toward long term vision
- Design, analysis, and fabrication of nanosystems will show us:
  - Technical barriers
  - New advances needed
  - Provide platform for future scaling