Sandia National Laboratories

SAND2013-0458P

LOCKHEED MARTIN


Exceptional Service in the National Interest

# National Labs and Production Sites


Sandia National Laboratories

# Sandia National Laboratories


Sandia National Laboratories

# Albuquerque details


Phoenix
1 hr air
6 hr car

<u>Albuquerque</u>
Population 800,000
University of New Mexico
Tech: 3 Intel fabs, 4 solar firms

Dallas
2 hr air

# Sandia National Laboratories -
## *over 200 UIUC Alumni strong*

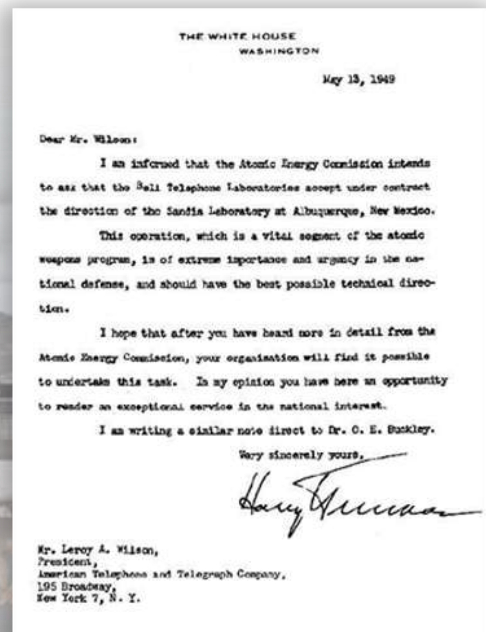
Amatucci, Vincent A
Anderson, Benjamin John
Anderson, Robert J
Ang, James A
Aragon, Alicia R
Arzigian, James S
Ashby, Carol I
Baldwin, Jon
Bieg, Kevin W
Borchardt, John Joseph
Boswell, Brad A
Boughton, Barry D
Bourdon, Chris J
Bowie, Jason
Branch, Darren Waltz
Brennecka, Geoff L
Bunker, Bruce C
Busick, Carla C
Carlson, David D
Carpenter, John H
Carroll, James F
Carroll, Malcolm S
Carter, Charles M.
Chen, Kuan
Choi, Seung J
Christensen, Gloria
Christensen, Jeffrey E
Christiansen, Gregory E
Chu, Dahlon D
Chu, Dahwey
Cich, Michael J
Clark, Blythe
Clem, Paul
Coltrin, Michael E
Condreva, Ken
Conley, William R
Coperich, Karen M
Copithorne, David
Corbet Jr, Thomas F
Crane, Nathan K
Cyr, Eric C
Davie, Neil T
Deland, Sharon
Dellinger, Jennifer
DeWitte, Michael D
Dixon, Dean A
Drotning, William D
Drummond, Timothy J
Duda Jr, Leonard E
Dvorack, Michael A
Dykhuizen, Ronald C
Elmazi, Nazim
Elmazi, Theckla
Eriksson, Timothy E
Euske, Jack
Evensky, David A
Farnum, Cathy Ottinger
Faust, Aleksandra
Field, Richard V
Fitzgerald, Russell Paul
Friedmann, Tom
Garino, Terry J
Gentile, Ann
George, Matthew
Gonzales, Antonio I
Griffiths, Stewart
Gronager, John E
Gross, Robert John
Gullerud, Arne S
Gupta, Vipin
Hafenrichter, Everett S
Hafenrichter, Thomas
Haill, Thomas A
Hales, Jason D
Hall, Aaron C
Handrock, Jim
Hapka, Michael Lee
Hardesty, Bonnie J
Harren, Ann
Hartwigsen, Christian J
Hatch, Steven W
Hattar, Khalid
Hebner, Gregory A
Heffelfinger, Steven R
Helfrich, Brian Edward
Helmich, Dennis R
Henderson, Craig
Hjalmarson, Harold P
Hoekstra, Robert J
Hosking, F Michael
Howerter, Christopher M
Hsu, Alan Y
Janssen, Curtis
Jiang, Jie
Jones, Reese
Jorgenson, Roy E
Jungst, Rudolph G
Kaneshige, Michael J
Kao, Gio K
Kaye, Ronald J
Kearney, Sean P
Kelly, Daniel P
Kempka, Steven N
Kent, Michael S
King, Tony L
Klem, John F
Klemme, Beverly
Konkel, Alexander
Kulp, Tom
Kuntz, David W
Laguna, George R
Laird, Daniel
Lappin, Allen R
Larson, Kurt
Lee, Ivan
Lee, Yun-ju
Lilly, Michael P
Lipinski, Ronald J
Liu, Johnson
Lober, Randy
Lott, Stephen E
Ludwigsen, John S
Mackey, Greg Edward
Mackoy, RD
Magee, Glen
Mahoney, Patrick
Manwaring, Scott Douglas
Matter, John C
Matzen, Laura E.
McClellan, H Lynn
McGovney, Gary N
Meisenheimer, Timothy L
Mendenhall, Frederick T
Merewether, Kimball O
Miller, Paul A
Miller, William M
Mills, Robert
Mitchell, Dean J
Myers, David
Noble, David
Novak, Jim L
Ollila, Eric
Olson, Rick
Padilla, Henry A
Pahl, Robert J
Papenguth, Hans W
Parks, Michael L
Pepping, Rick
Petti, Jason P
Goudy, Sue P
Pierson, Kendall Hugh
Pontau, Art
Pott, John
Randall, Gary T
Reichardt, Thomas
Renschler, Cliff
Resor, Brian R
Ringland, Jim
Robles, Jennifer
Rosenthal, Mark A
Roskovensky, John K
Roth, Peter
Rothganger, Fredrick
Ruffolo, Marisa
Sault, Allen G
Savignon, Daniel J
Schaefer, Mark A
Schiek, Richard L
Schoenwald, David A
Sears, Mark P
Sempsrott, Jason
Serrano, Justin Raymond
Siefert, Christopher
Skala, Dawn
Skocypec, Russell D
Slezak, Scott E
Snow, Clark S
Soo Hoo, Mark S
Spahn, Olga Blum
Spulak, Robert G
Stewart, James R
Stygar, William A
Sutton, Katherine E
Talischi, Cameron
Tang, Jason D
Taylor, Paul A
Ther, David T
Tuttle, Bruce A
Vanderheiden, Margaret M
Varma, Sameer
Vaughn, Andrew
Vernon, Milton E
Villanueva, Rose Q
Wagner, Kenneth Charles
Walther, Howard P
Warren, Drake E
Watson, Robert D
Weber, Thomas M
Weiner, Ruth
Wierer, Jonathan
Wilkening, Lisa K
Wilson, Rodney K
Winrow, Edward G
Wyss, Gregory
Yang, Pin
Yarrington, Paul
Young, Michael F

Sandia National Laboratories has one of the largest concentrations of University of Illinois alumni of any company outside the state of Illinois, with University of Illinois grads from Chemistry, Chemical Engineering, Mechanical Engineering, Civil Engineering, Physics, Nuclear Engineering, TAM, Biophysics, ECE, CS, Mathematics, Astronomy, Geology, Ceramic Engineering, Materials Science, Metallurgical Engineering, and more.

Sandia National Laboratories

# Heritage

***"Exceptional service in the national interest"***



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

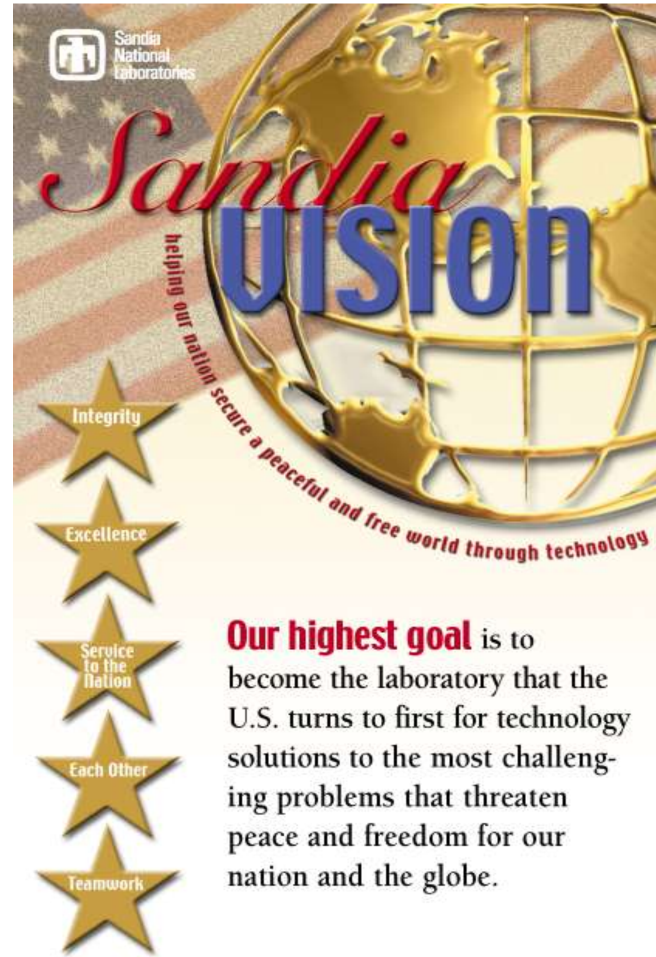
Very sincerely yours,

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.



# Exceptional Service in the National Interest

- **National Security Laboratory**
- **Broad mission in developing science and technology applications to meet our rapidly changing, complex national security challenges**
- **Safety, security and reliability of our nation's nuclear weapon stockpile**



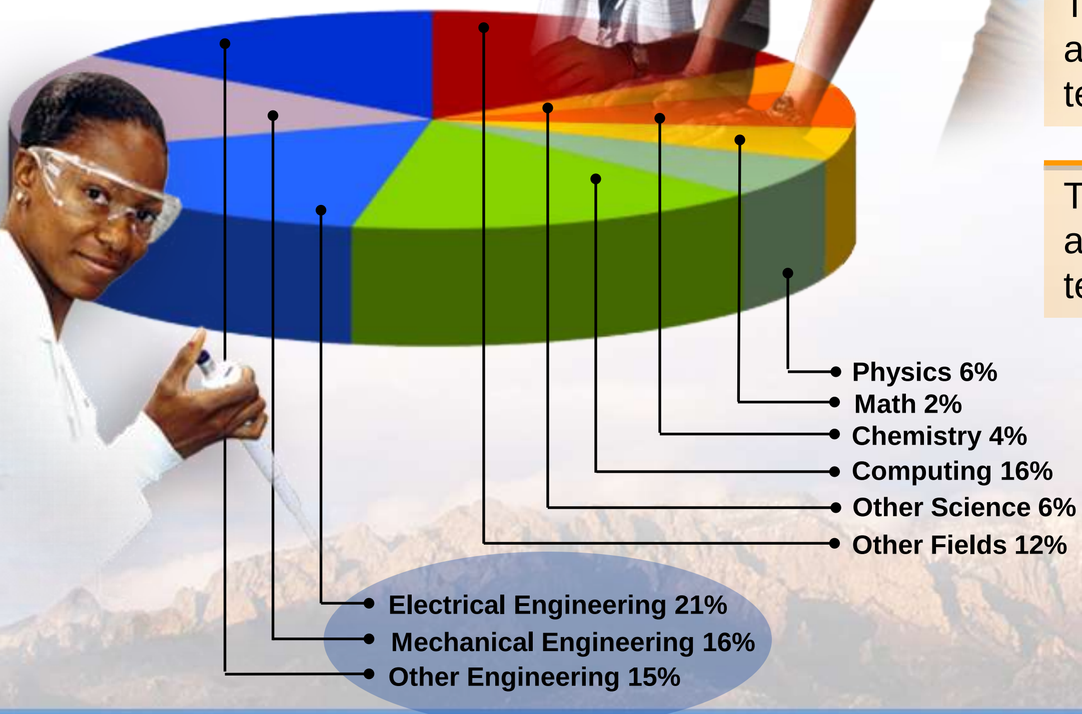
# Shaping Sandia's strategic path through objectives and goals

- Deliver with excellence on our commitments to the unique nuclear weapons mission.
- Amplify our national security impact.
- Lead the complex as a model 21st century government-owned contractor-operated national laboratory.
- Excel in the practice of engineering.
- Commit to a learning, inclusive, and engaging environment for our people.

# Sandia's People

- **On-site workforce: 11,677**
- **FY10 permanent workforce: 8,607**
- **FY10 gross payroll: $898.7M**
- **FY10 budget: $2.3B**

**Technical Staff (4,277) by Degree**
(End of FY10)




**Disciplines of Most Technical Hires**
(FY06 – FY09)

| | |
|---|---|
| Top 3 hire fields comprise approximately 52% of technical hires | ▪ CS/CE<br>▪ EE<br>▪ ME |
| Top 5 hire fields are approximately 68% of technical hires | ▪ Chemistry<br>▪ Physics |
| Top 10 hire fields represent approximately 82% of technical hires | ▪ Nuclear Eng<br>▪ Geo & Environmental Sciences<br>▪ Bio/Biochem<br>▪ Materials Science<br>▪ Math |

Sandia National Laboratories

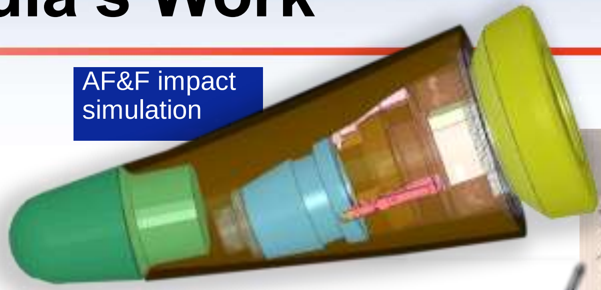
# Sandia's Work

Shuttle Orbital Inspection System

## 4 Mission Areas

- Nuclear Weapons
- Defense Systems and Assessments
- Energy, Resources, and Nonproliferation
- Homeland Security and Defense

Predator UAV with SAR



AF&F impact simulation

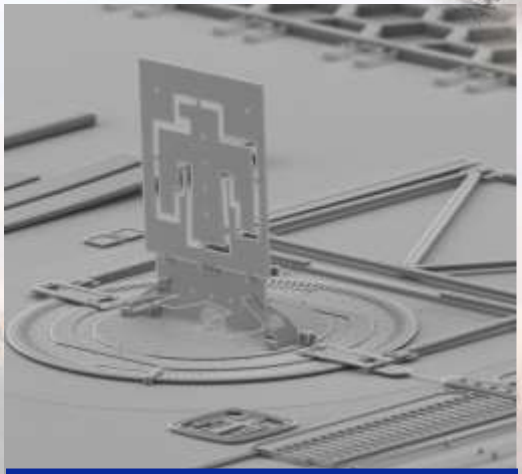
96% of total NW parts

Small robotic vehicles

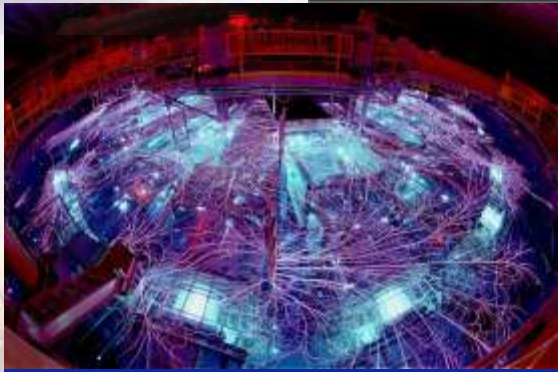
UGS

Renewable and alternative energy

µChemLab



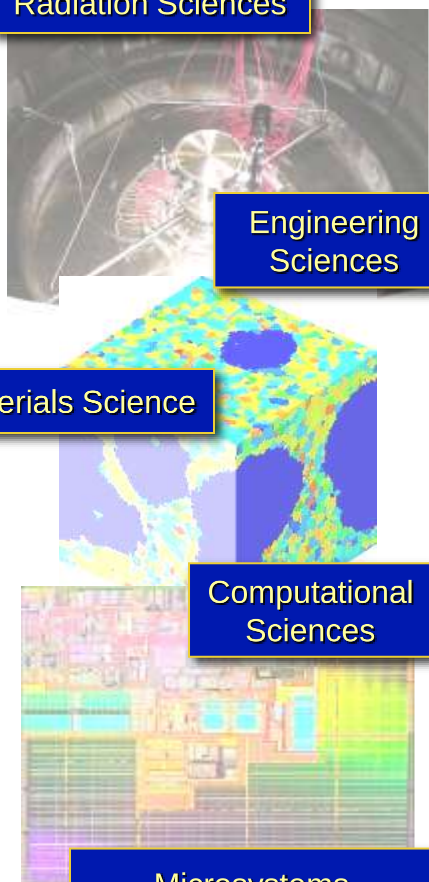
Clean room invented at SNL in 1963



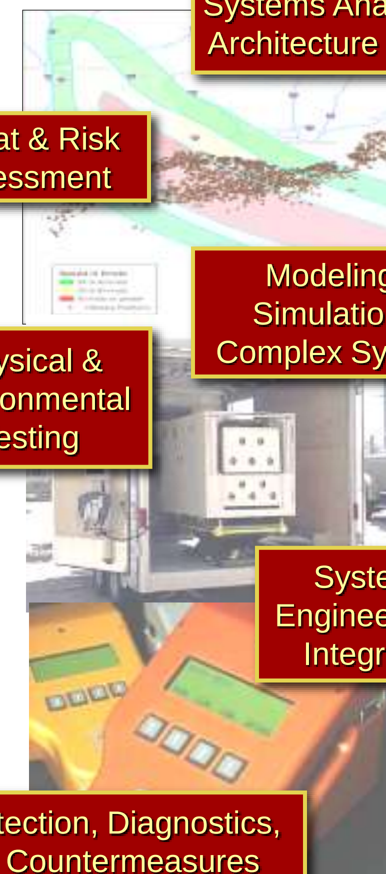
Z machine:
the world's most powerful X-ray source

# Core Capabilities

S&T Research Foundations + Relevant Special Facilities = Homeland Security Capabilities







# Sandia's strategic capabilities are underpinned by 6 research foundations

## Strategic Capabilities

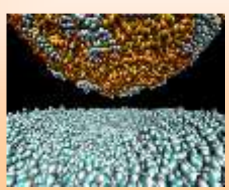
High Performance Computing & Simulation

Nanotechnologies and Microsystems

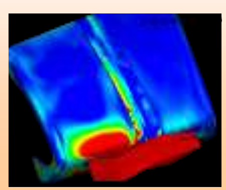
Extreme Environments

Computer Science

Materials

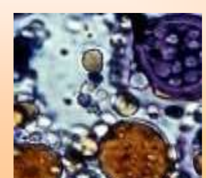


Engineering Sciences



Micro Devices

Bioscience



Pulsed Power

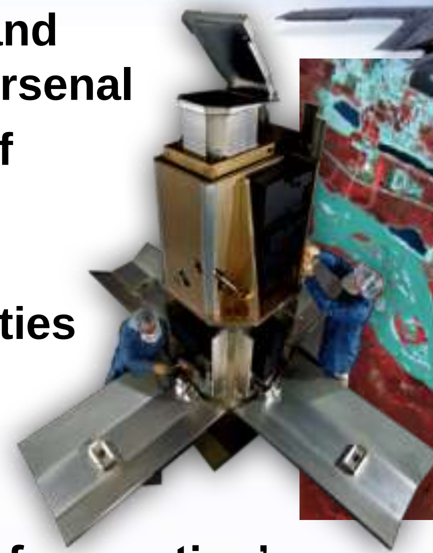
## Research Foundations

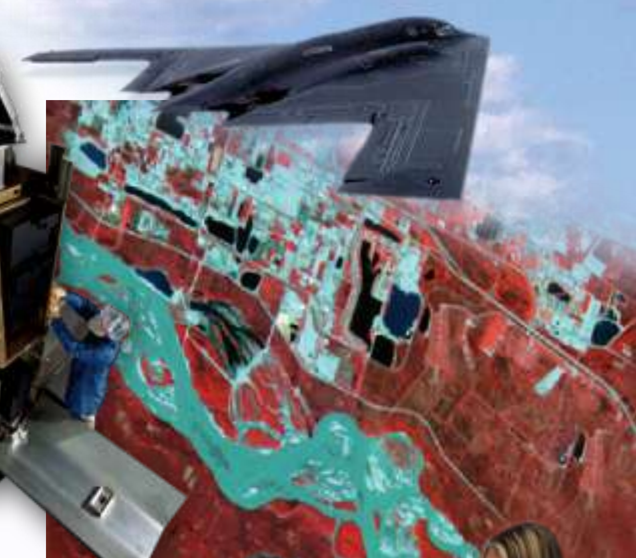
# Sandia’s Unique Set of Resources

- World's largest x-ray source
- World's smallest chemical and biological analysis systems
- Tallest solar tower in the United States
- First clean room
- First MEMS in space
- World's largest center for fundamental and applied study of combustion processes
- World's largest federal investment in microsystems technology
- One of the world's fastest general-purpose supercomputers
- World-class team of engineers, chemists, physicists, biologists, mathematicians . . .

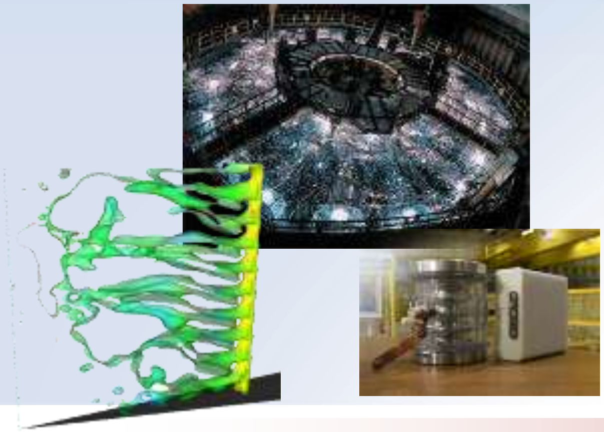
# Technologies for National Security

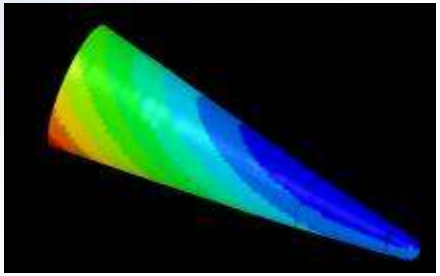
- We develop technologies to:
  - Sustain, modernize and protect our nuclear arsenal
  - Prevent the spread of weapons of mass destruction
  - Provide new capabilities to our armed forces
  - Protect our national infrastructures
  - Ensure the stability of our nation’s energy and water supplies.
  - Defend our nation against terrorist threats

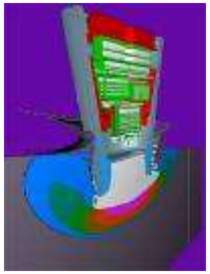




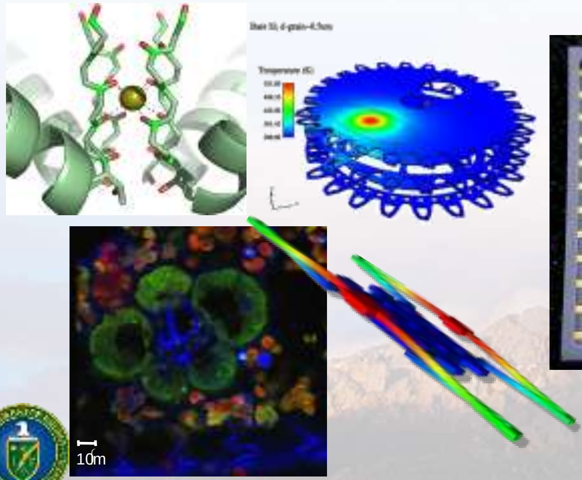
# Materials Science is Critical Throughout

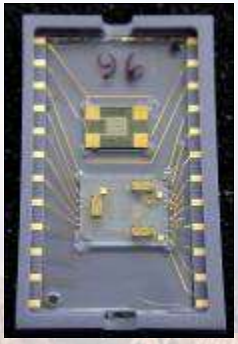


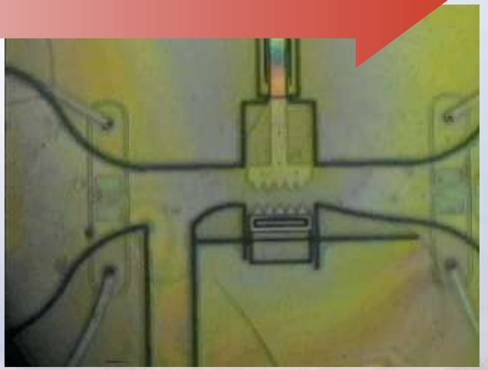




***From Atoms to Systems***

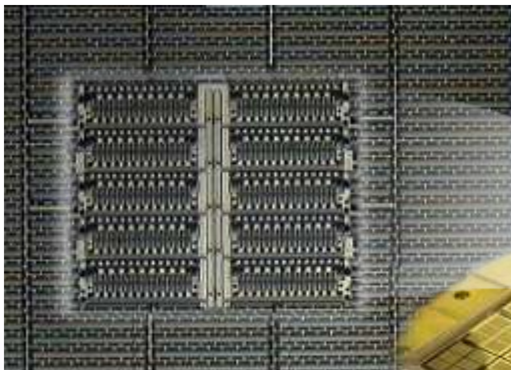


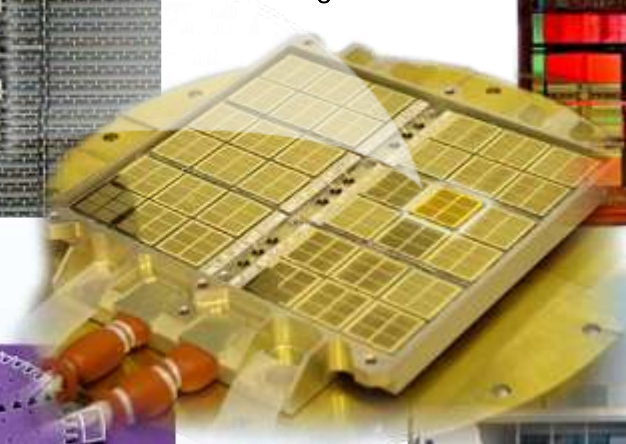


# Capabilities: Microsystems

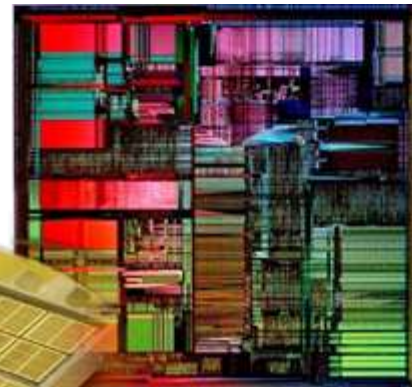
MEMS louvers manufactured at Sandia



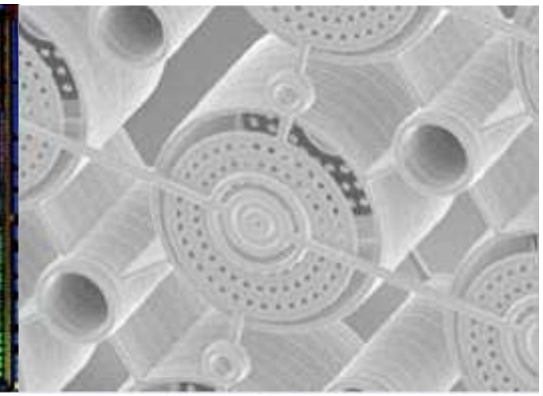
Johns Hopkins/APL thermal regulator



Application-specific integrated circuit



Ion traps for quantum computing

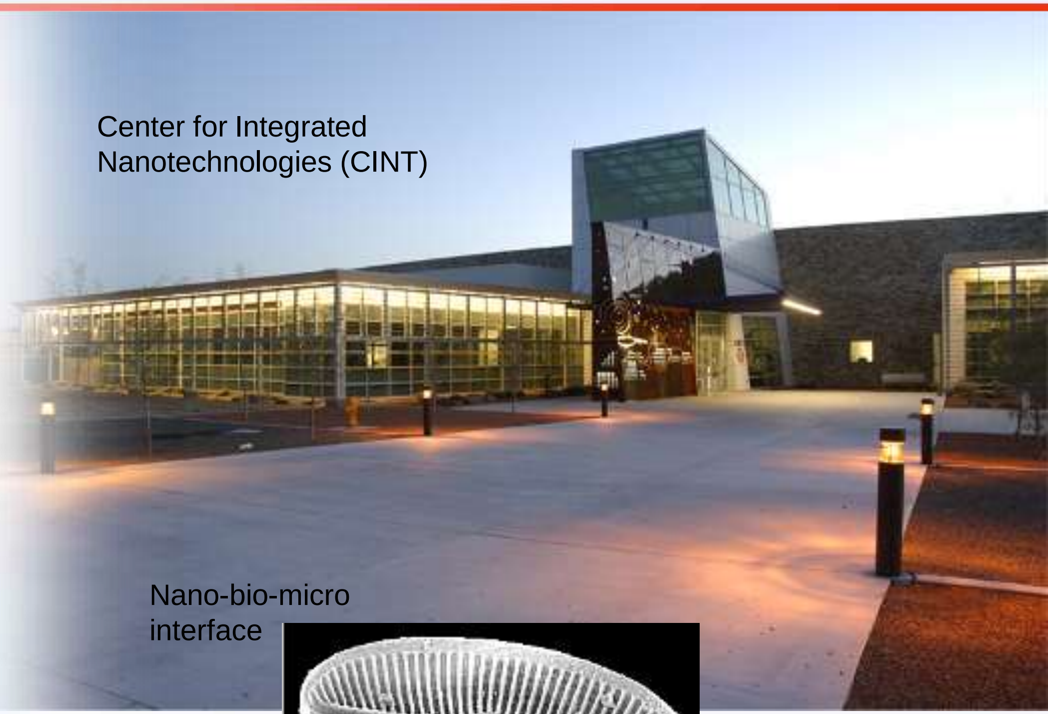


Microgears

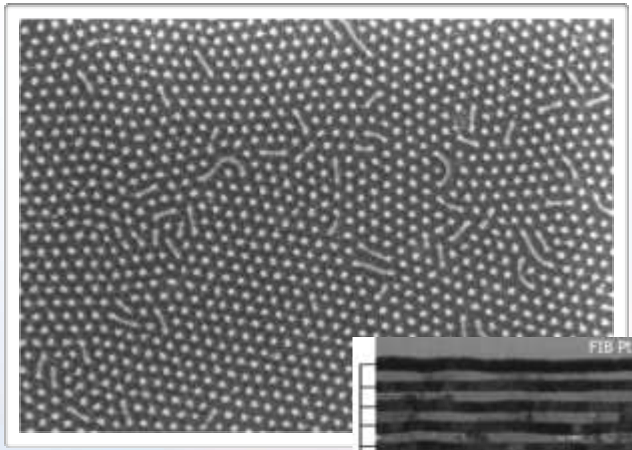
Outside view of the Microsystems Engineering for Strategic Applications (MESA) and clean room at MESA

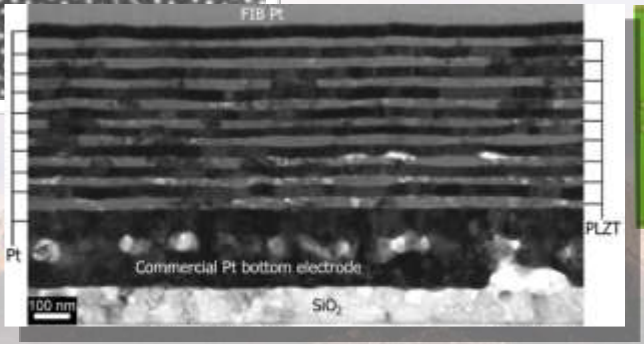
# Capabilities: Nanotechnology

Complex functional nanomaterials

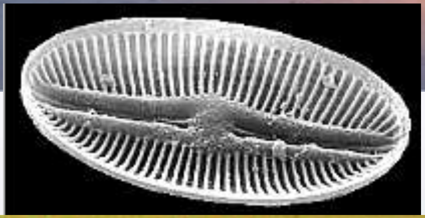


Center for Integrated Nanotechnologies (CINT)

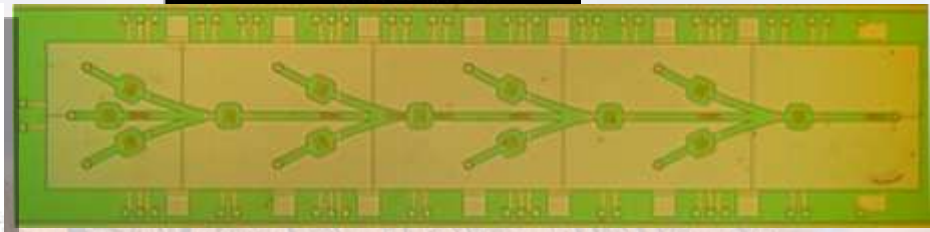





Nano-bio-micro interface



Microfluidic chip



# Exploring Solutions Across the Threat Spectrum

# Sandia captures four R&D 100 awards

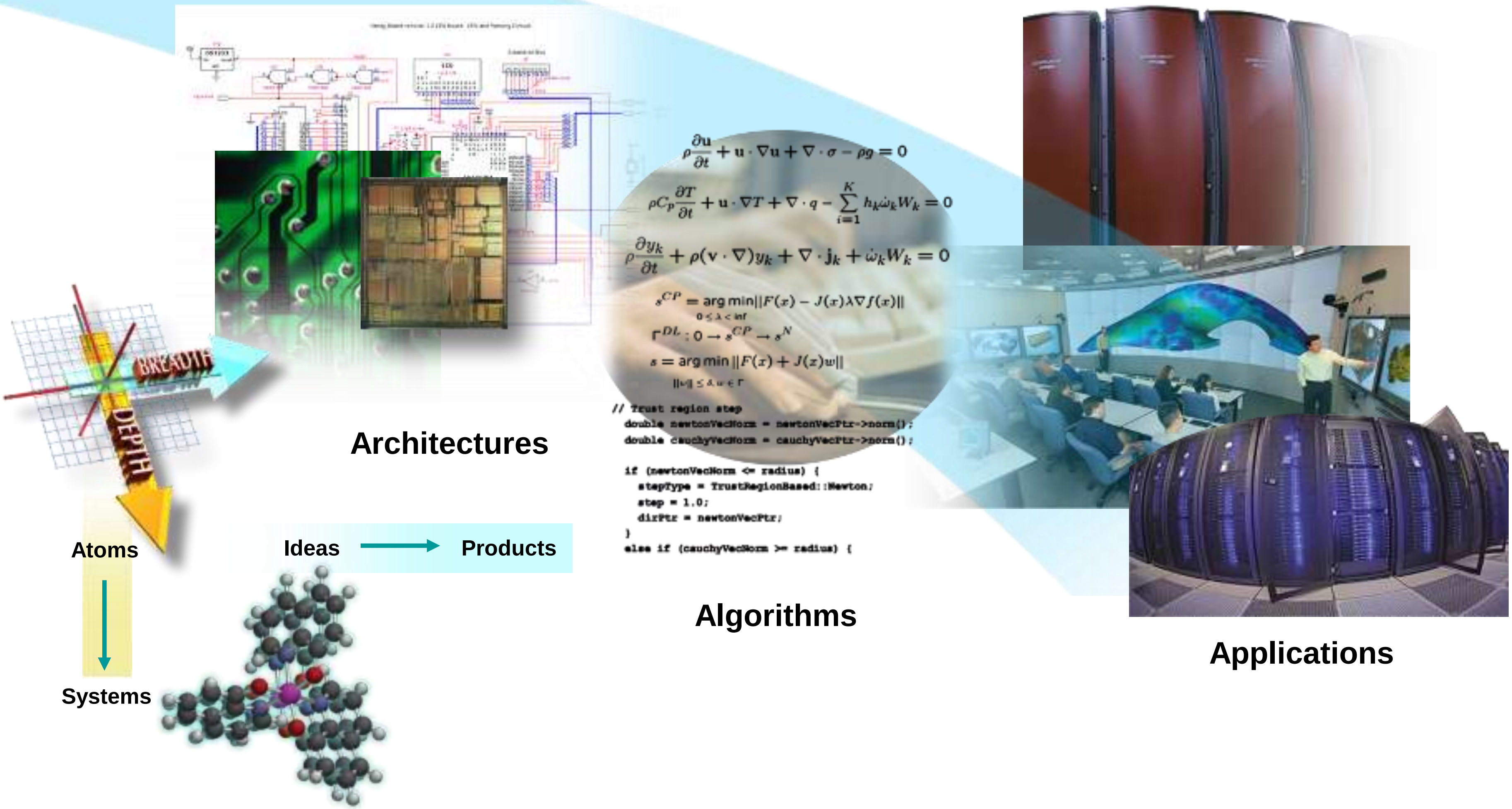
*And the winners are . . .*

- Microresonator Filters and Frequency References
- Ultra-high-voltage Silicon Carbide Thyristor
- Biomimetic Membranes for Water Purification
- The Demand Response Inverter (Sandia is a co-winner on this entry)

# Vision for Transforming Computational Science and Engineering

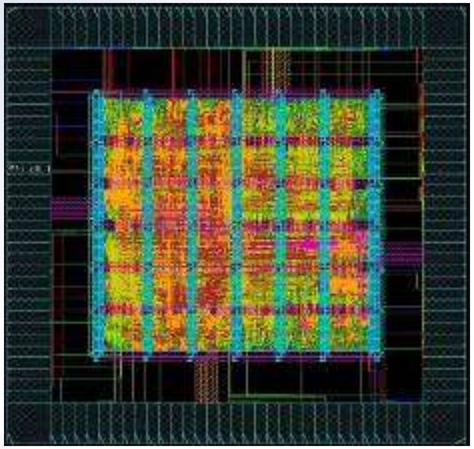
**One 1994 computer day ≈ One 2006 computer minute**

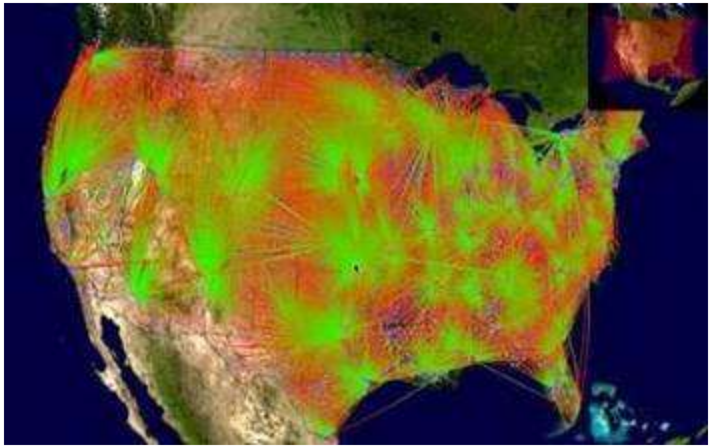
**1997: 1 Teraflop in a *room.* 2007: 1 Teraflop on a *chip.***



# Science & Technology for Cyber Security

Low Power
Cryptographic Chip





Infrastructure modeling

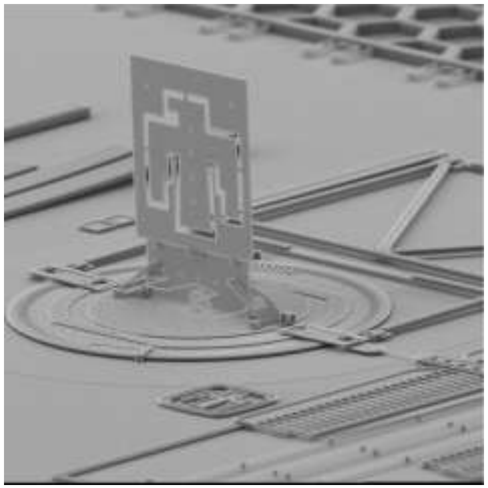

Identification of genuine
versus counterfeit parts

Microelectronics
Development Lab
(Trusted Foundry)

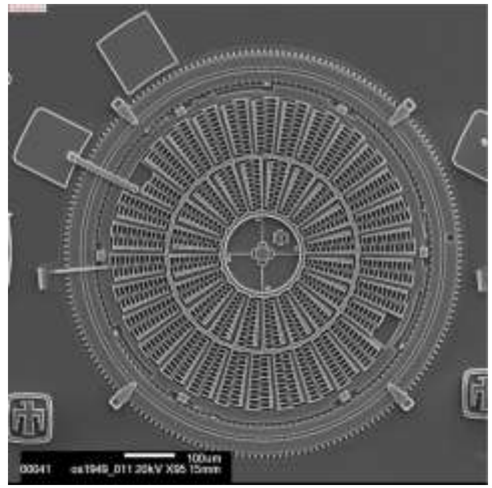
http://mems.sandia.gov/

# Sandia MEMS

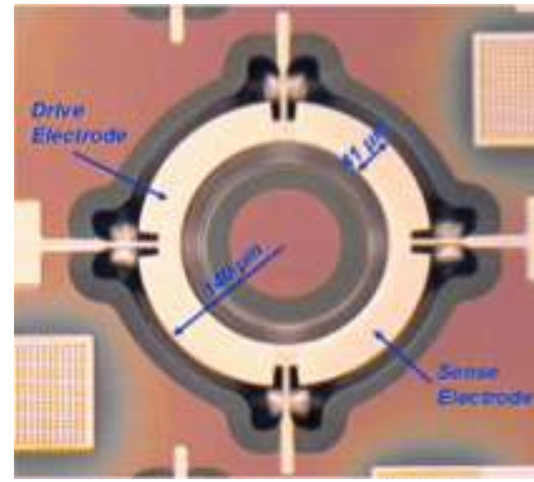
µElectroMechanical



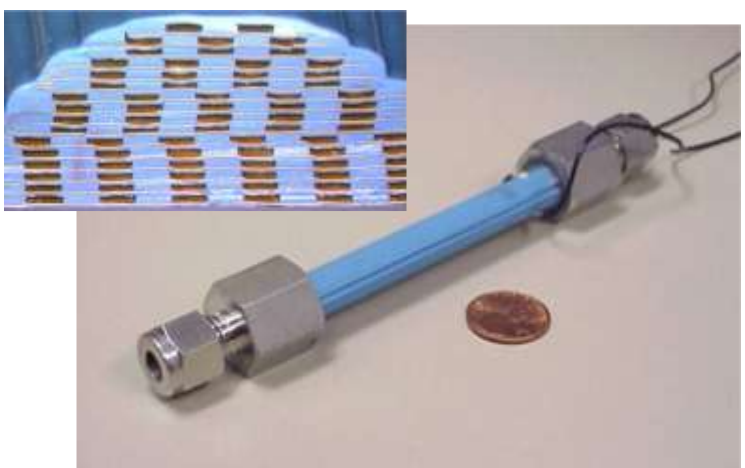
Torsion Actuator



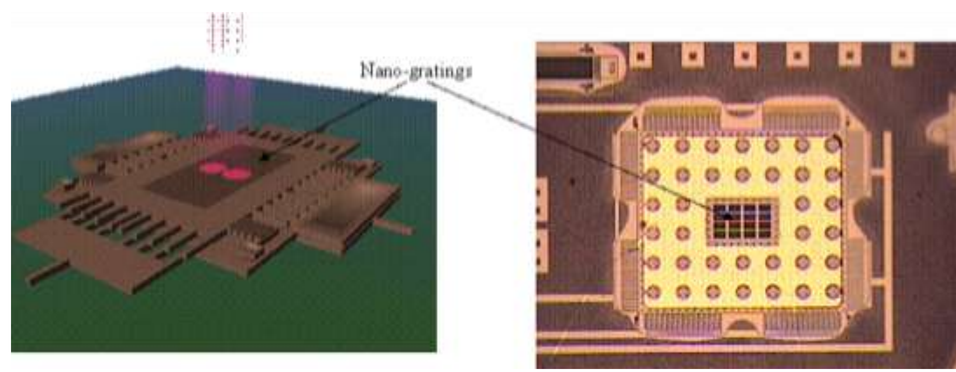
RF MEMS




BioMEMS/µFluidics

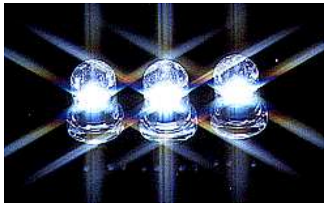


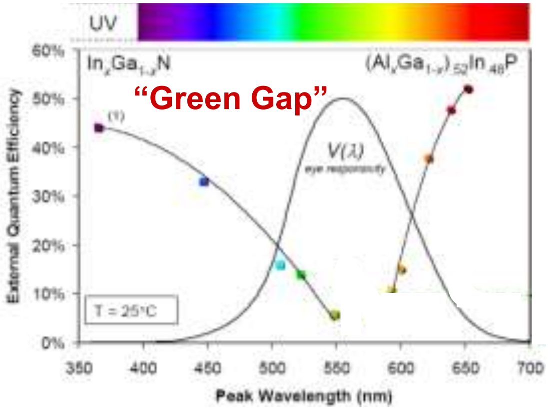
Nano-grating based Low-G inertial sensor

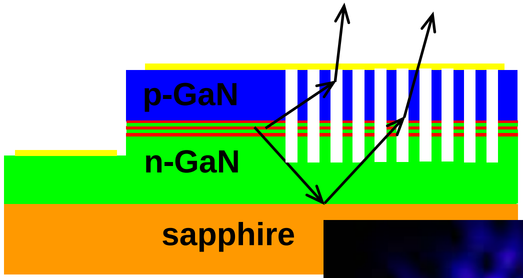


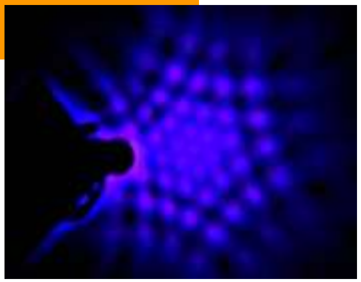
# Solid State Lighting

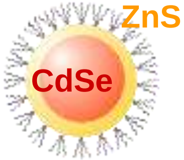
- If 2025 Solid-State Lighting 50% efficiency goals are met, U.S. electricity consumption will be reduced by 10%, saving > $25B/ year
- Sandia's activitives
- – State-of-the-art materials growth
- – Seeking solutions to major materials and LED challenges
- – Advanced light extraction concepts
- – Novel white light generation approaches
- Courtesy of Mary Crawford

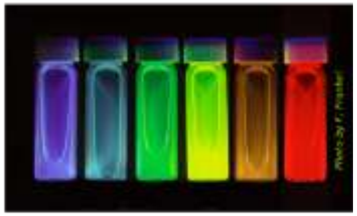


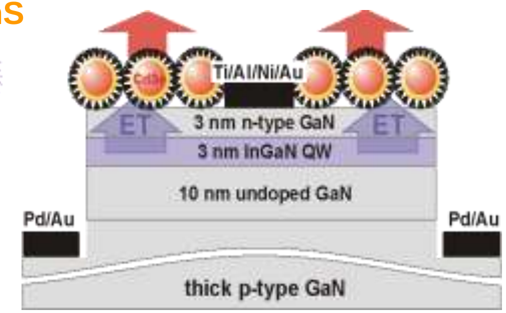




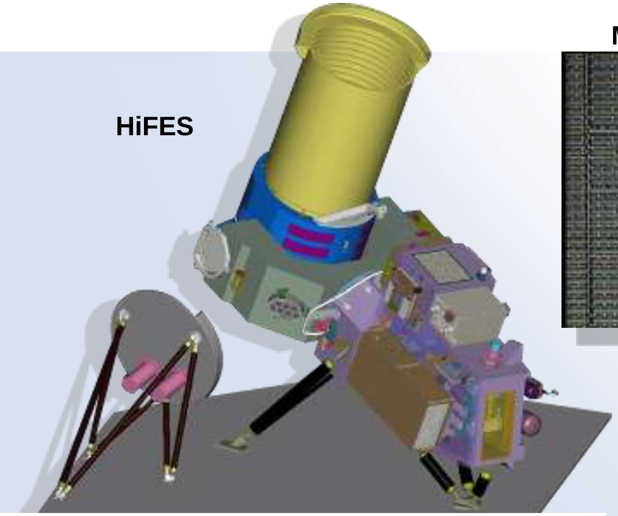





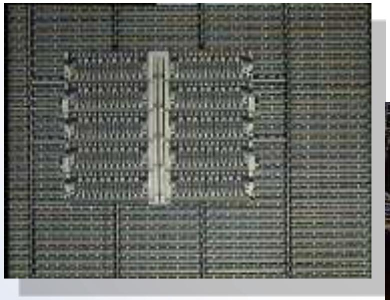

collaboration with LANL

# Science & Technology for Space

HiFES



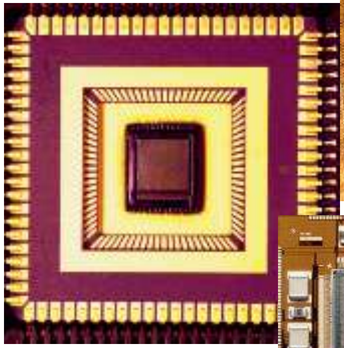
MEMS louvers



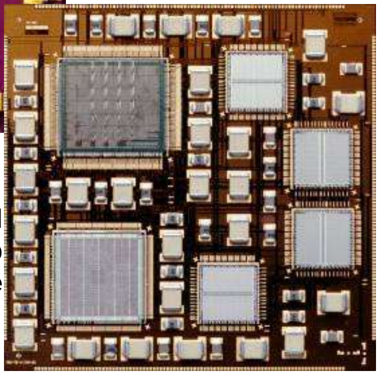
Laser Dynamic Range Imager Orbiter Inspection System (LOIS)

Galileo spacecraft

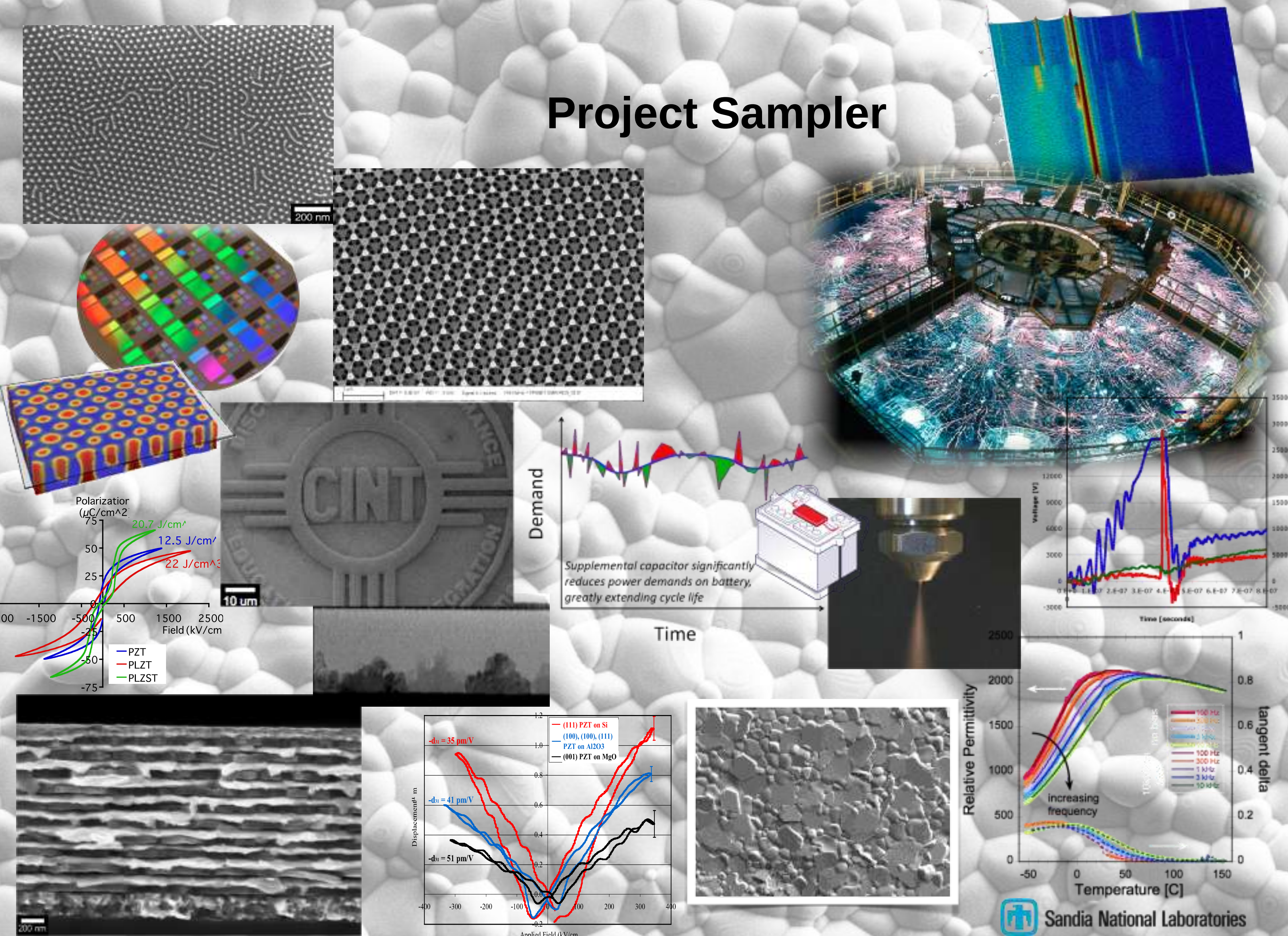
Focal plane array



Rad-hard multi-chip module

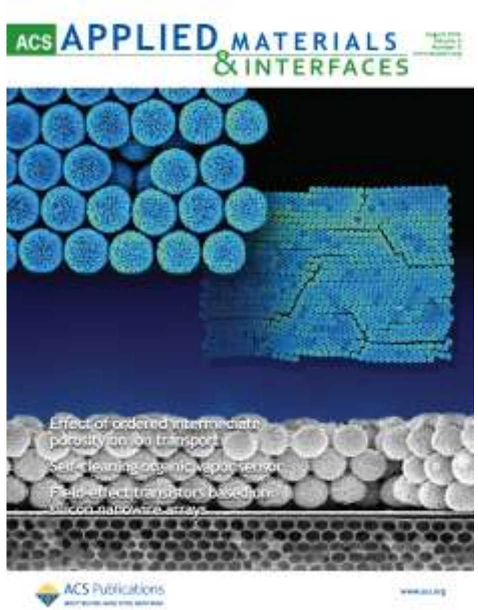


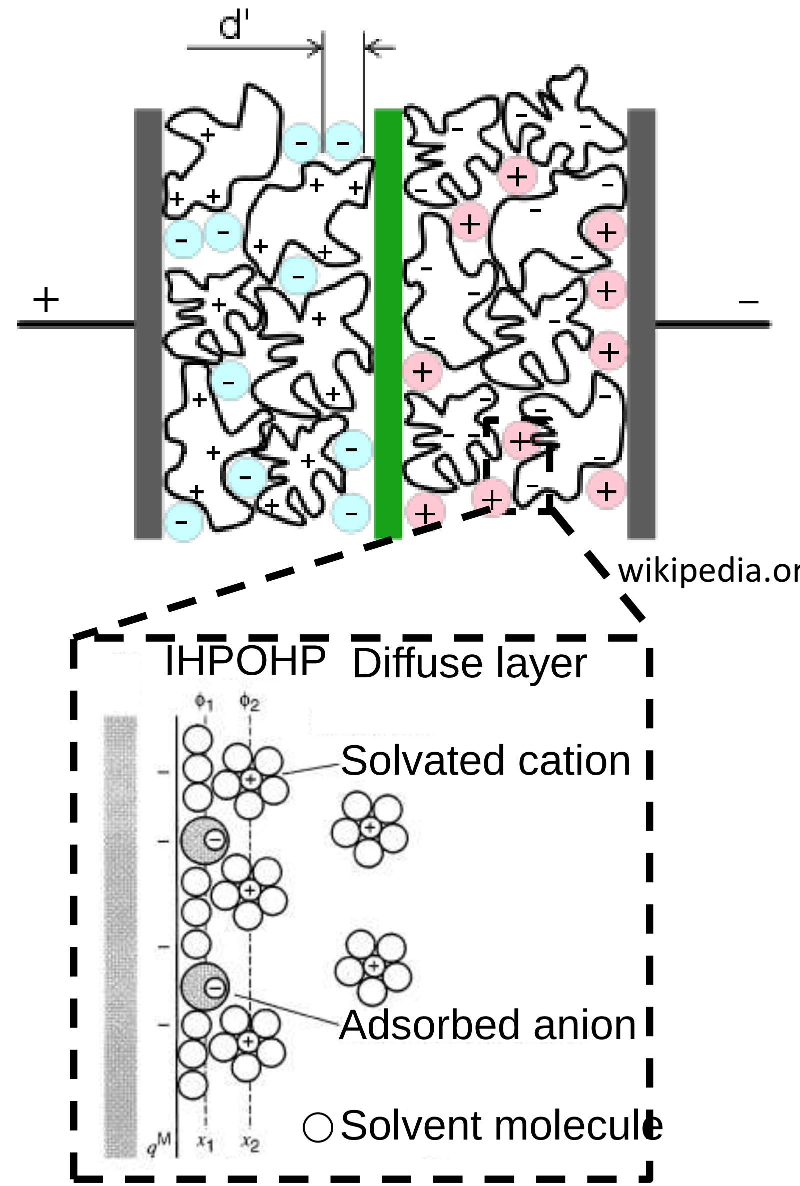
# Project Sampler

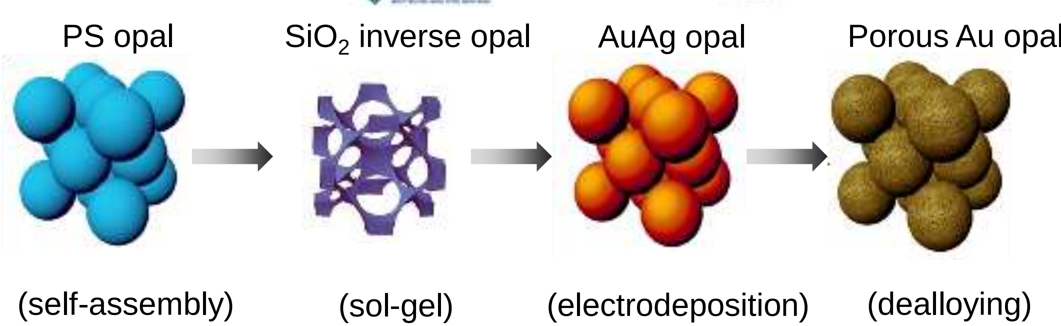


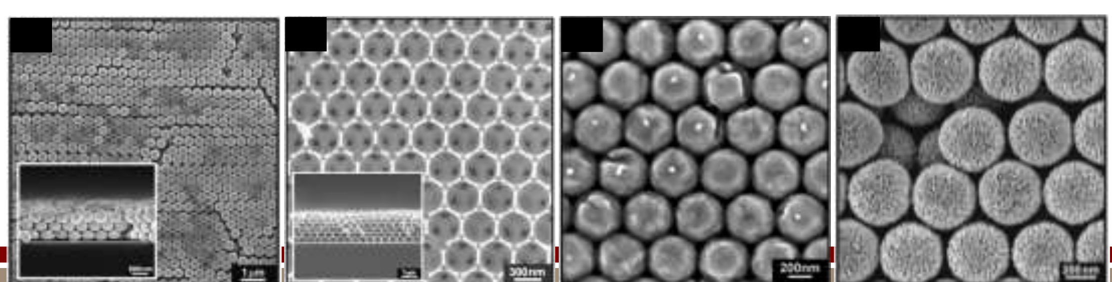
# Hierarchical porous EDLC electrodes

Collaboration between Sandia & University of Illinois




D.V. Gough et al. ACS Applied Materials & Interfaces (2012)

# *In situ* Ion Irradiation Capabilities

350 kV implanter

100 kV nanoimplanter

6 MV tandem accelerator

3 MV pelletron accelerator

- Newest and Highest Energy in situ TEM ion irradiation facility
- Developing it to be the first concurrent in-situ TEM

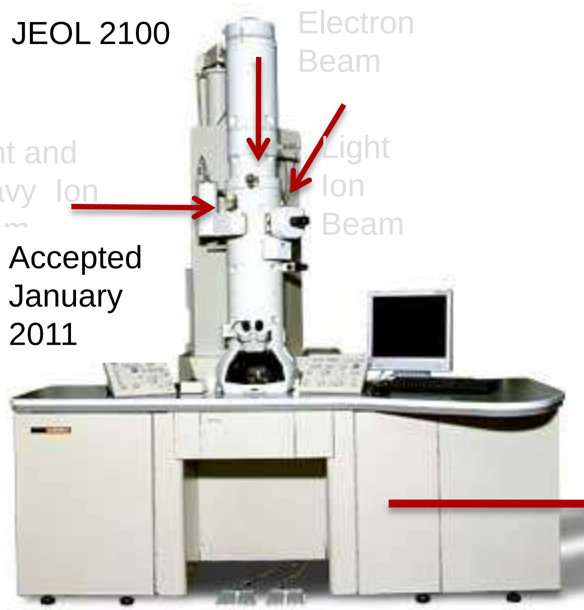
200 kV TEM attached to 6 MV tandem

# *In situ* Ion Irradiation TEM

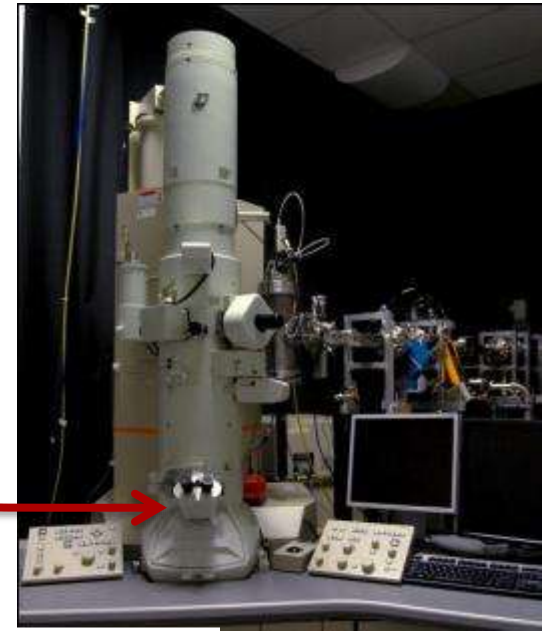
## Proposed Capabilities

- 200 kV $LaB_6$ TEM
- Ion beams considered:
  - 3 MeV $He^{1+}$ $Si^{3+}$ $Cu^{3+}$ $Au^{3+}$
  - 14 MeV $Si^{3+}$
  - 10 keV $D^{2+}$
  - 10 keV $He^{+}$
  - All beams will hit same location
- Electron tomography
- Nanosecond time resolution (DTEM)
- Procession scanning (EBSD in TEM)
- *In situ* PL, CL, and IL
  - Optical pathway purchased
- *In situ* heating and cooling stage
- *In situ* electrical measurement stage
- *In situ* straining stage
- *In situ* vapor phase stage
- *In situ* li

JEOL 2100

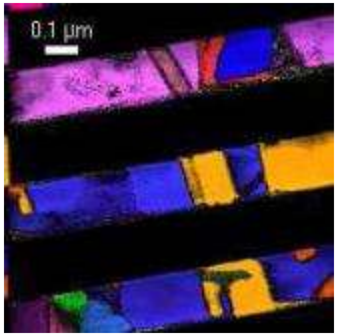



Accepted
January
2011



TVIPS

Hummingbird




Nanomegas

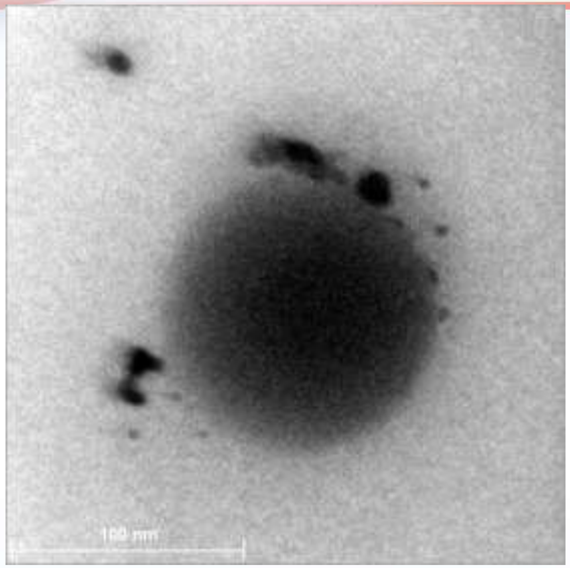
We have completed the 1st generation (Tandem Accelerator) and have initiated building the 2nd generation (Colutron Accelerator). Many potential additions are being considered

# Exciting New Directions in *in situ* TEM

## Protocell Drug Delivery

S. Hoppe,
D. Sasaki,
E. Carnes,
J. Brinker

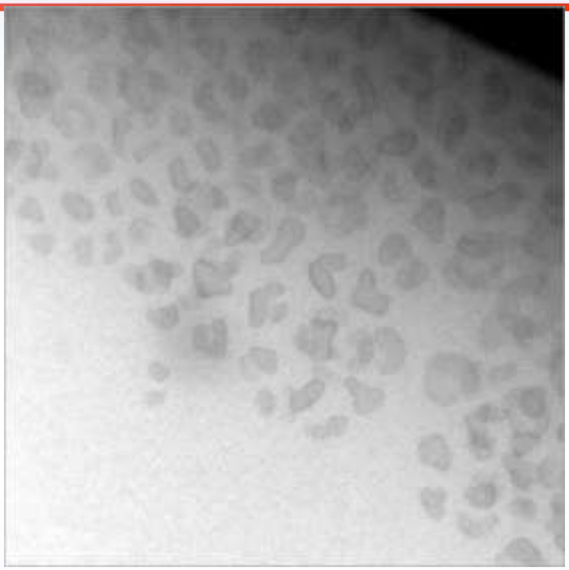
Liposome encapsulated Silica destroyed by the electron beam




## BSA Crystallization

S. Hoppe

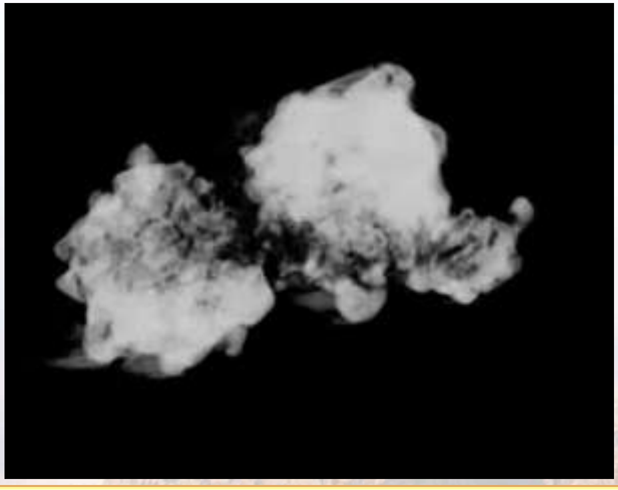
Crystallization of excess Bovine Serum Albumen during flow



## Tomography of Pd NP

B. Yates,
J.V. Branson
D. Robinson

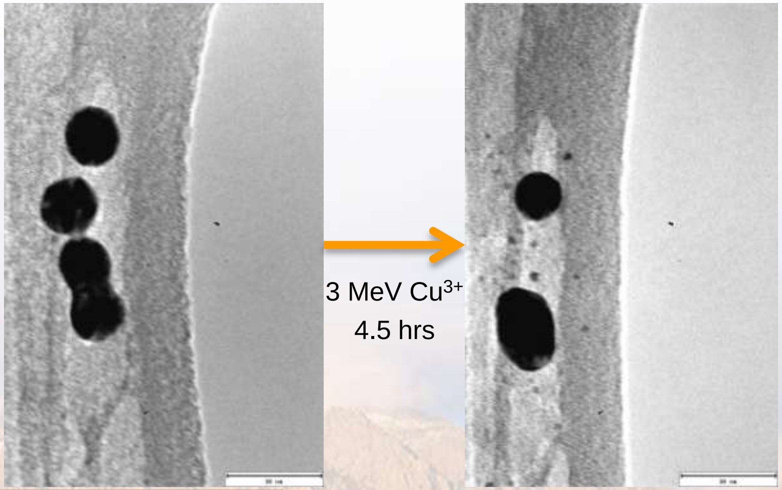
Porous Pd nanoparticles reconstructed in 3D



## Ion Irradiation of Au NP

S. Hoppe,
S. Rajasekhara

Sintering and sputtering of Au nanoparticles during ion irradiation




**The combination of new capabilities permit better understanding at the nanoscale of systems in real environments**

Sandia National Laboratories

# Working Environment at Sandia

- People: professionals mostly, 15% postdocs, 10% students
- Large number of females, few non-US citizens
- Flexible work hours: 9/80, half time
- All projects are team-oriented; very few single investigator projects

Raising Money

- Sandia: Present day diverse funding portfolio (NW, BES, DOD, industry, intelligence)
- High overhead, comparable to industry
- > 20% of my time dealing with funding (proposal, networking, meetings, reports)
- Majority of Sandians work on assigned projects & do not need to raise his/her money

# Student Internships

## Institutes

- Physical Sciences Institute
- Computer Science Research Institute
- Center for Cyber Defenders
- Enabling Predictive Simulation Research Institute
- Sandia Institute for Modeling and Simulation
- National Security Engineering Institute

## Internships and Co-ops

- **Year-round and summer**
- **Must be a U.S. citizen with full-time enrollment status**
- **Minimum cumulative GPA of 3.2/4.0 for undergraduates or 3.5/4.0 for graduate students**
- **STEM and business disciplines**
- **Apply online at Sandia's website: www.sandia.gov**
- **Pay based on job classification and the number of academic credit hours completed prior to internship**

# Finding a position

1) Provide resumes to Sandia UIUC recruiters
   khattar@sandia.gov
   dgough@sandia.gov

- Apply online: http://www.sandia.gov/careers

- Network at Professional Meetings

common criteria:

- field of expertise
- research experience/publication record
- GPA

# Contrast with Academic Careers

| National Labs | Academia |
|---|---|
| R&D for national needs | Educate next generation |
| Colleagues, professionals | Students, postdocs |
| Top down management, teaming | Individual groups (no boss) |
| US capability, safety & security focus | Technical results focus |
| Flexible work schedules/ career paths<br>- 40 hr week vs. 9/80 (every 2nd Friday off)<br>- technical staff ladder vs. technical manager | Tenure clock, funding cycles<br>- independence<br>- high time expectations |
| Team projects | Individual PI |
| Raise money | Raise money |
| High starting pay but leveling out to uniform | Low starting pay but large variation at full professor |

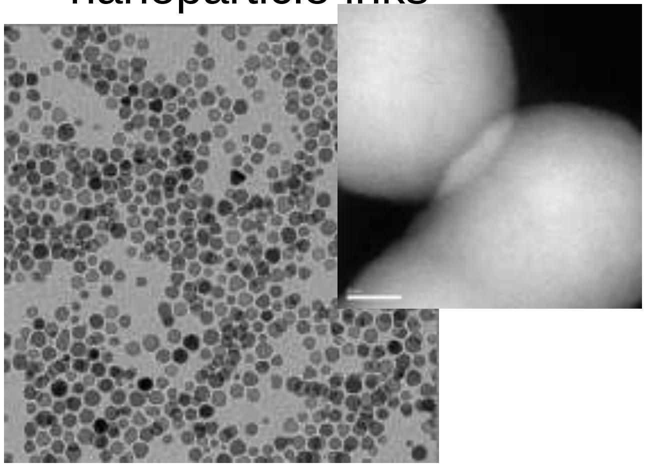
# Contrast with Industrial Careers

| National Labs | Industry |
|---|---|
| R&D for national needs | R&D for one company |
| Colleagues, professionals | Colleagues, professionals |
| Top down management | Top down management |
| US capability, safety & security focus | Profit focus |
| Flexible work schedules/ career paths | Meet deadlines, milestones, quarterly |
| Raise money to do what you want | Funding is directed; might help write group proposals |
| High starting pay but leveling out to uniform | High starting pay but leveling out to uniform |

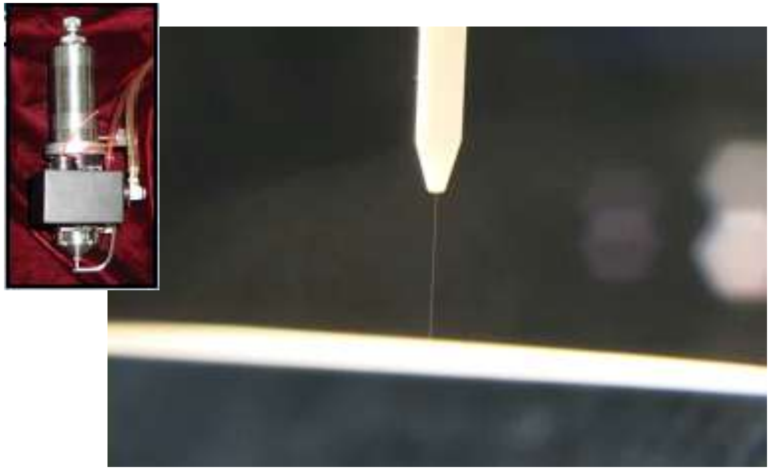
# Direct-Write Fabrication

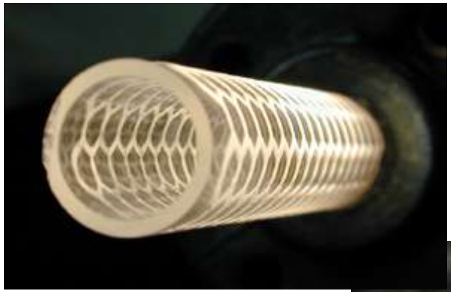
- Useful on curved surfaces, flexible substrates (polymer, textile), & 3D structures
- Sandia technology
– Several methods
– 10-25 µm lines
– Various (Ag, Au, Pt, Cu) nanoparticle inks
– On curved surfaces
- Courtesy of Paul Clem

nanoparticle inks



Aerosol microspray jet



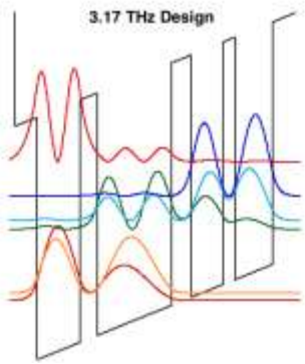


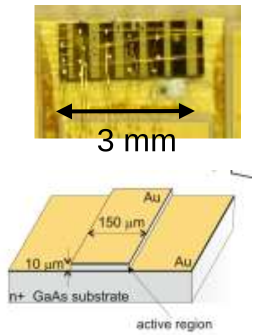
3D Antenna

Thunderbird on Mylar balloon

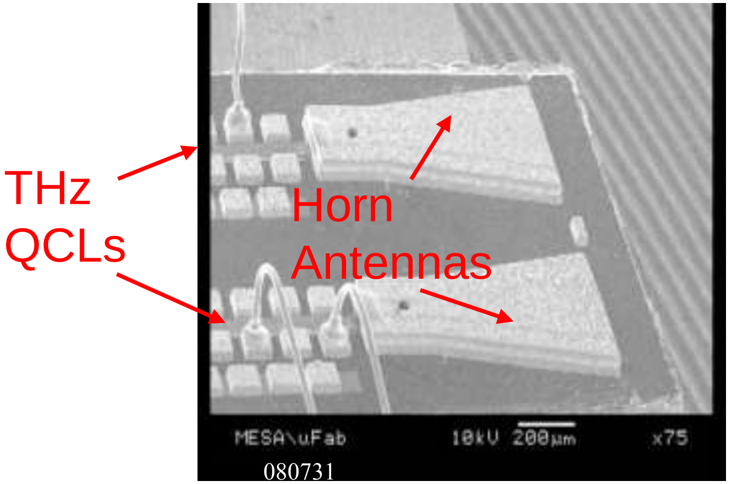
# THz Research

## Quantum Cascade Lasers



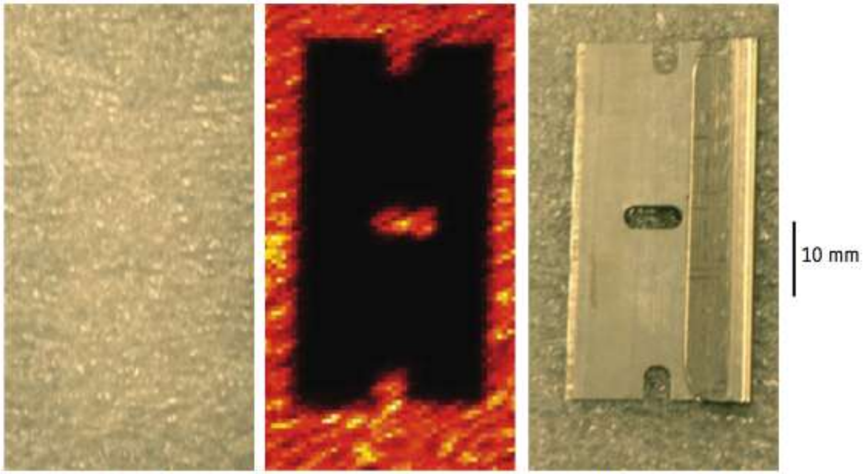




## On Chip Integration




## Seeing Behind the Wall (Superman)


(a few mW)




Front of thick packing foam

"See-through" image as seen using a 2.9-THz QCL

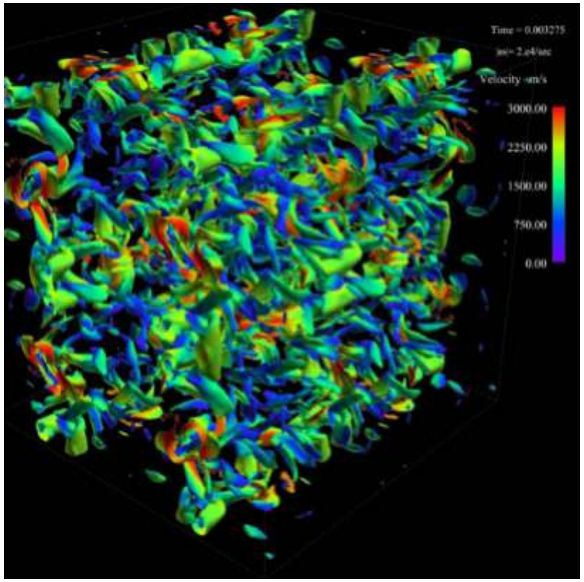
The real image in the back of the packing foam

Courtesy of Mike Wanke & Igal Brener

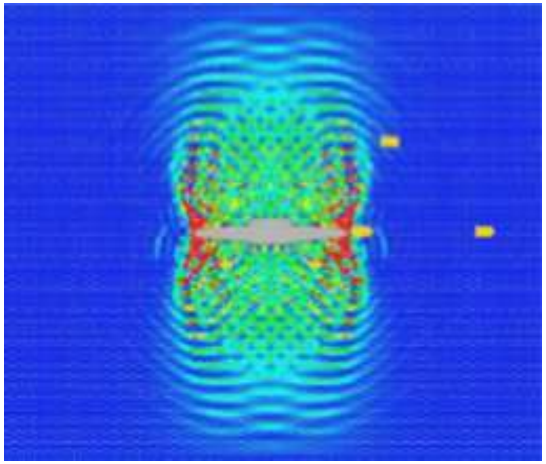
# Advanced Simulation and Computing

- Supports Defense Programs' shift in emphasis from test-based to simulation-base confidence
- High Performance Computing (HPC)
– Sandia: Red Storm
– Los Alamos: Roadrunner
– Livermore: BlueGene/L
– Commercial: IBM, Cray
- [http://www.sandia.gov/NNSA/ASC/](http://www.sandia.gov/NNSA/ASC/)

Red Storm




Penetration and production of x-rays and electrons inside weapon systems from the radiation of hostile nuclear encounters and space environments.



Fracture mechanism: micro-crack propagation in materials

# High Speed Testing

Rocket Sled Track Facility provides a controlled environment for high-velocity impact, aerodynamic, acceleration, and related testing of small and large test items.

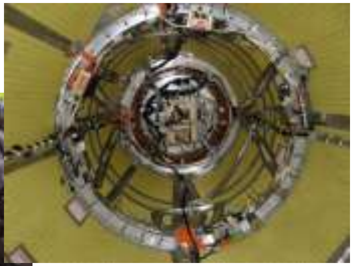
- 10,000-foot track for high speed testing and 2,000-foot railroad gauge track for large items
- High-speed video, flash x-ray, and film cameras running 40,000 frames per second and higher; also, on board recording
- Max acceleration: 100g, Max speed: M3

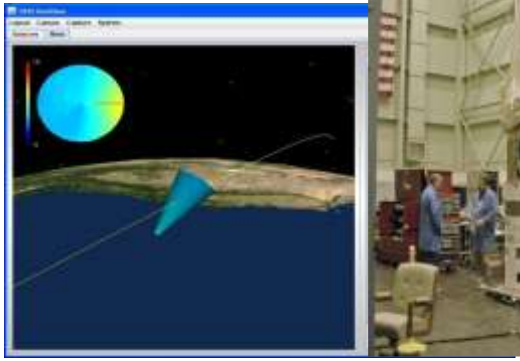
full-size F-4 aircraft traveling at 700 ft/s impacts a 350-ton concrete abutment to test the strength of the concrete for use in a nuclear power facility

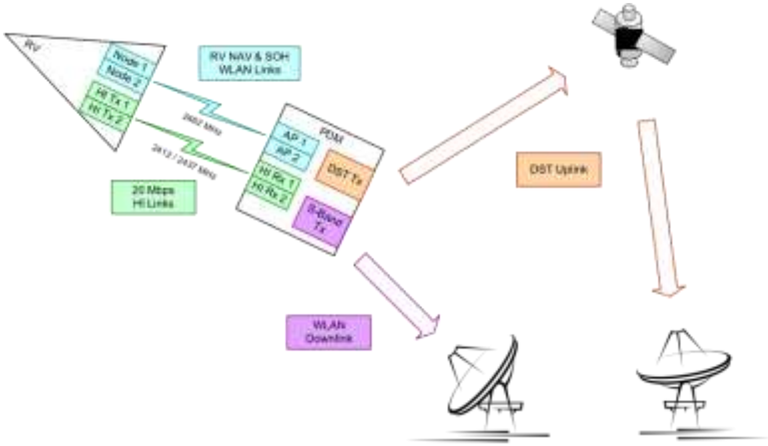
3.2 ms after detonation during a 4,000 ft/s sled test

# Target Flights

- Telemetry and Instrumentation
  - RV, Payload Deployment Module, Countermeasures
- Real Time Data Analysis and Visualization
- Advanced Development
  - Wireless LAN
  - Virtual Ground Station
  - Satellite Communication
- Courtesy of John Vonderheide





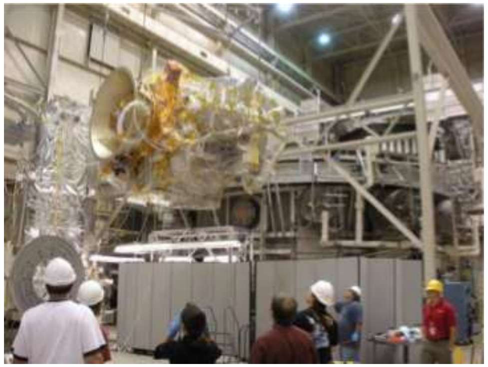


# Launch Targets

Sandia-operated missile test sites in Hawaii, Alaska and Nevada

# NASA
# Lunar Reconnaissance Orbiter (LRO)

- First Moon Mission since the 70’s
- Scheduled to launch on 4/29/2009
- Objectives: find safe landing sites, locate potential resources, characterize the radiation environment, and test new technology
- Sandia contributions
  - provided the digital transmitter and receiver for the SAR (Mini-RF) payload
  - after NASA scans the surface of the moon, reconfigure these elements to function as an experimental communication link for future lunar missions (made possible by Sandia’s unique technology)
- Courtesy of Scott Holswade



# Who is leading globally in energy research…

## Energy & Fuels:

Institutions Ranked by Citations

| Rank | Institution | Citations 1998-2008 |
|---|---|---|
| 1 | Sandia National Labs | 4,147 |
| 2 | Natl. Renewable Energy Lab | 3,773 |
| 3 | CSIC (Spain) | 3,678 |
| 4 | Chinese Academy of Sciences | 3,541 |
| 5 | Indian Institutes of Technology | 3,166 |

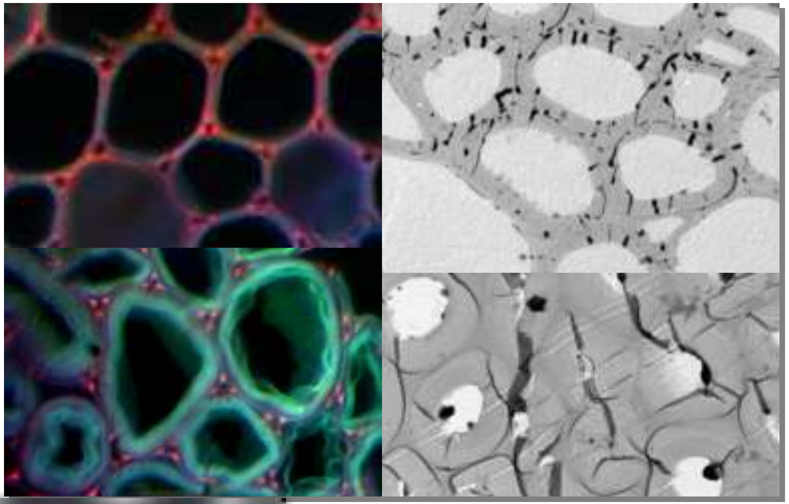
*Source: Thomson Reuters Science Citation Index*

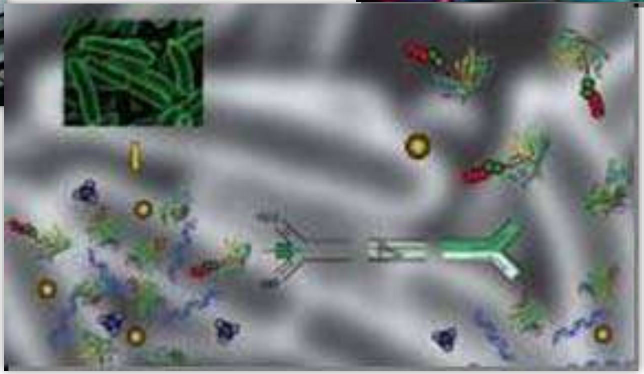
- **U.S. national labs lead the way**
- **National labs and U.S. universities comprise 9 of the top 20 research institutions**
- **Sandia is 1st in total citations of energy and fuels research and 3rd in papers cited in photonics research.**

# Joint BioEnergy Institute (JBEI)

*"Advancing the Development of the Next Generation of Biofuels"*

JBEI is a $135M joint Research Center now moving to Emeryville, CA location





"Lab-on-a-Chip" technology to enhance enzyme purification and analyses

Pursuing more efficient switchgrass saccharification
- Cost-effective lignocellulose pretreatment
- Identify new microbes to produce lignocellulose enzymes

# Renewable Energy Research

## Wind

- **Next Generation Wind Turbines**
  - **Improve Energy Capture by 30%**
  - **Decrease Capital Costs by 25%**
  - **Improve Reliability**

## Solar

- **Improved Performance Through**
  - Manufacturing Process Improvements
  - Harnessing Nanostructures
  - Thermal Storage Materials and Systems

# Nuclear Energy

*"Renew U.S. leadership in 'Nuclear Energy' . . ."*

## National Technical and Policy Leadership

- Yucca Mountain Project License Application
- Safety and Security
- Transportation
- Repository Science

## Nuclear Fuel Cycle Science

- Advanced Fuel Cycle Technologies
- Advanced Modeling and Simulation

## Key System Demonstrations

- Nuclear-Solar Hydrogen
- Small Reactor Development
- International Fuel Return Demonstration
- Transparency Technology Demonstration

# Carbon Capture: Motivation & Targets

“Rapid commercial development and deployment of clean coal technologies, particularly carbon capture and storage, will help position the United States as a leader in the global clean energy race.”

President Barack Obama

“To prevent the worst effects of climate change, we must accelerate our efforts to capture and store carbon in a safe and cost-effective way. This funding will both create jobs now and help position the United States to lead the world in CCS technologies, which will be in increasing demand in the years ahead.”

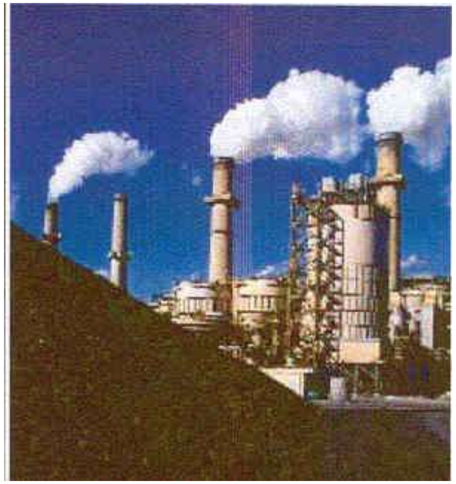
- Energy Secretary Steven Chu

*$CO_2$ emission from* *coal-fired electric power* *is:*

- *>1.5 x $10^9$ metric tons (>1.5 GT)*
- *predicted to grow to > 2GT/year by 2020*

*Removal goal is: 1 GT/year (1 $km^3$ of liquid $CO_2$)*

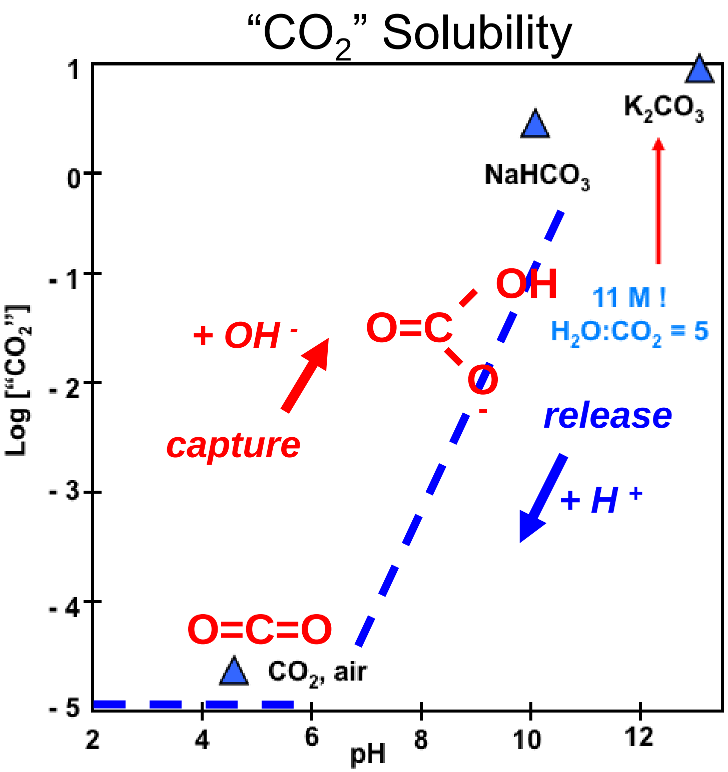
*Desired cost of $CO_2$ capture: $10/metric ton*

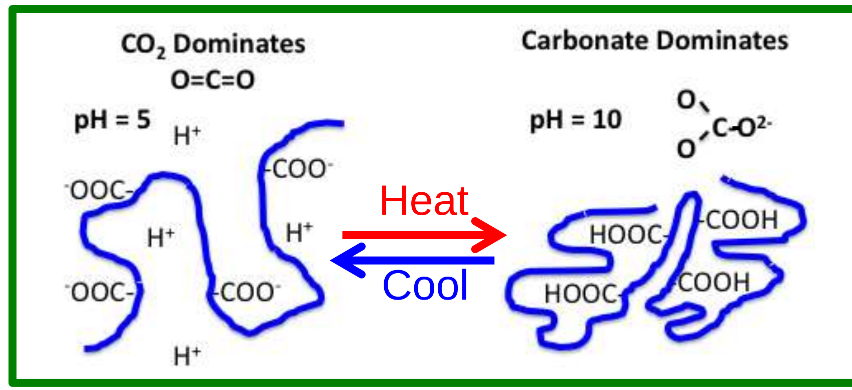


**Processes must be selective, reversible, cheap, and capable of handling billions of tons of $CO_2$, preferably from air.**

DOE/NETL Carbon Dioxide Capture and Storage RD&D Roadman (Dec 2010); www.netl.doe.gov

# Programmable Materials for $CO_2$ Sequestration

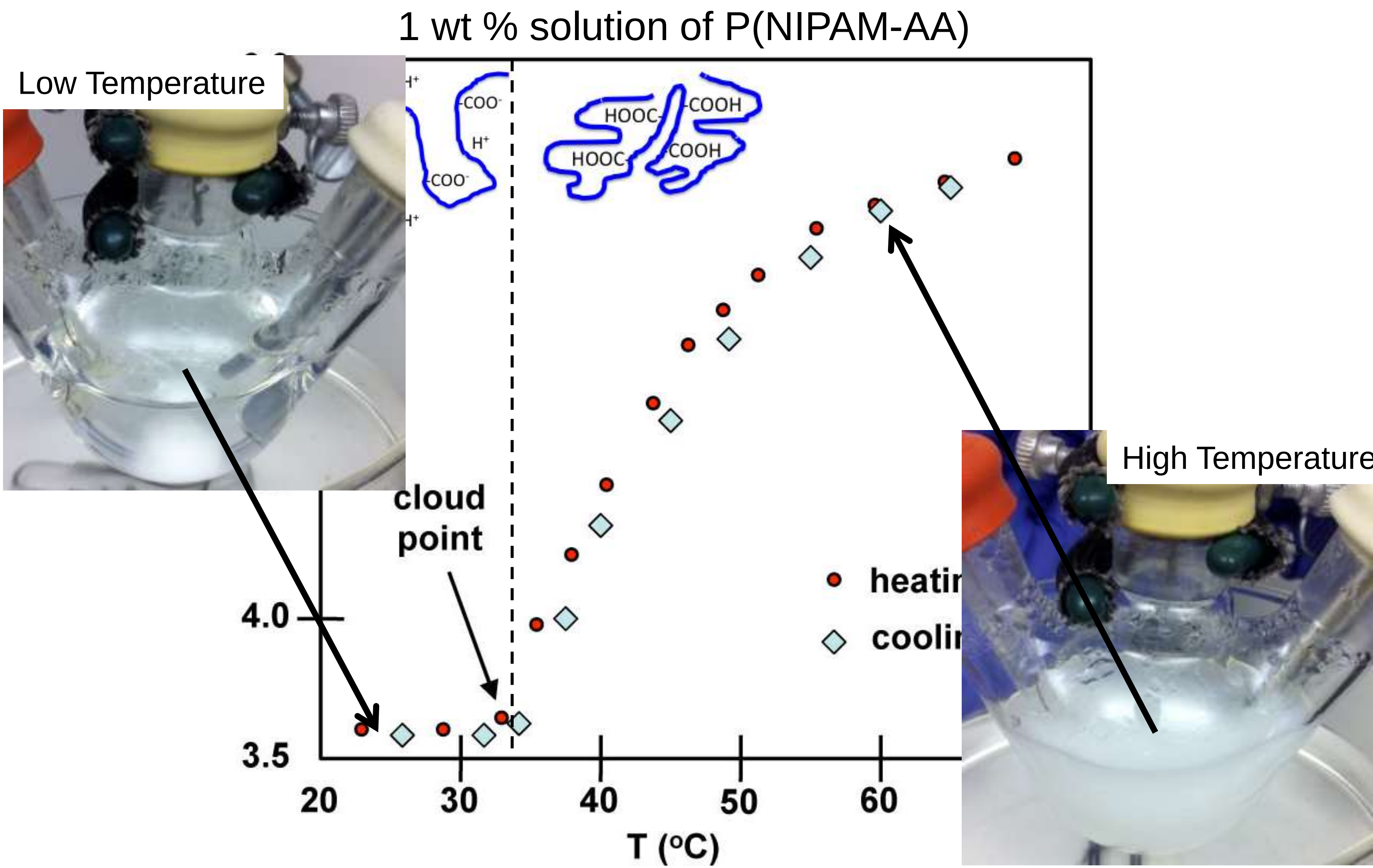



1) The transition induces large, reversible changes in solution pH.

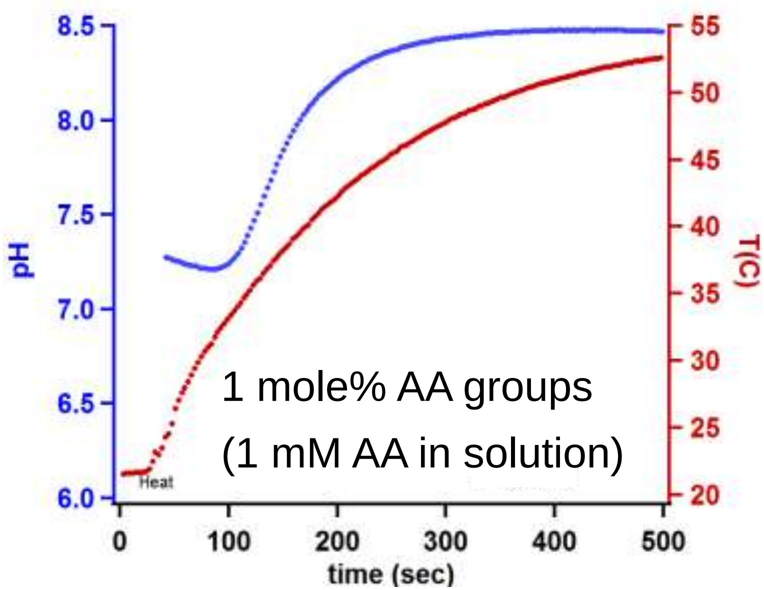
*2) Programming of the polymer should suffice for loading/unloading of $CO_2$.*

# Programmable Materials for $CO_2$ Sequestration

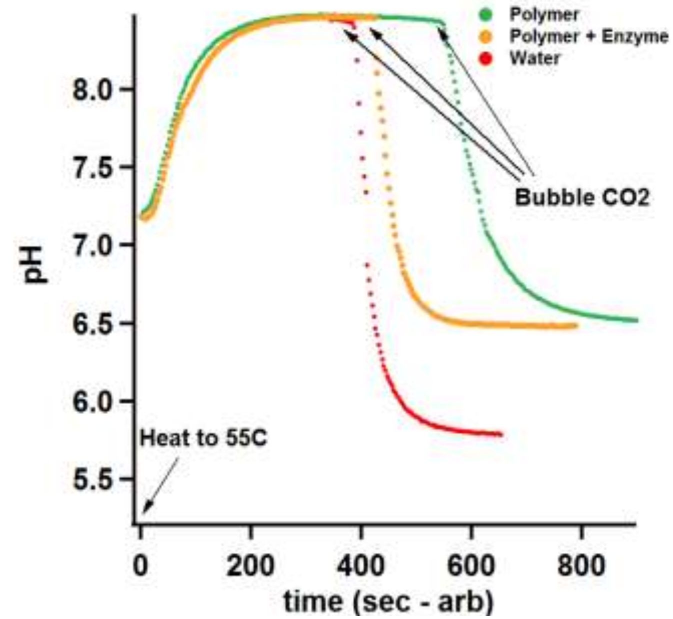


# Captured [$CO_2$] Increases with Temperature

Sandia National Laboratories



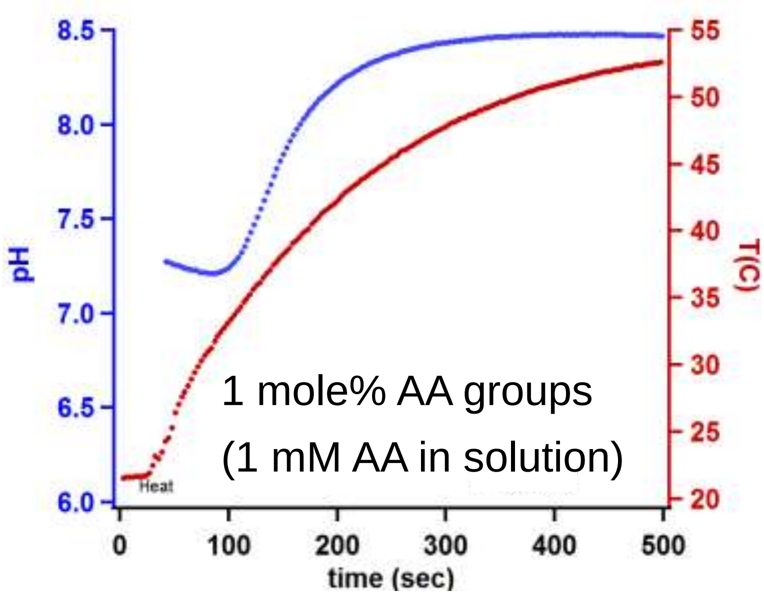

Thermally programmable pH change about neutral pH using acid groups ($pK_a$ = 5)!



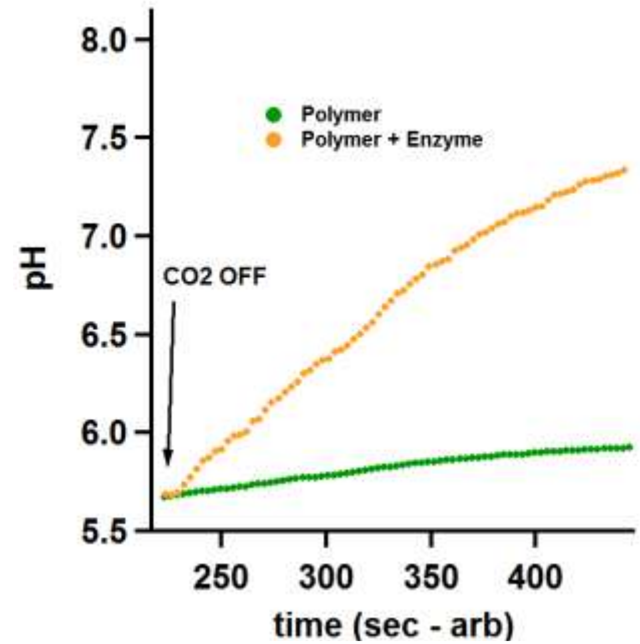

$CO_2$ capture for polymers in high temperature configuration

Taking advantage of the copolymer pH behavior increases capacity by 55%!

# $CO_2$ Release Upon Cooling




Thermally programmable pH change about neutral pH using acid groups ($pK_a$ = 5)!



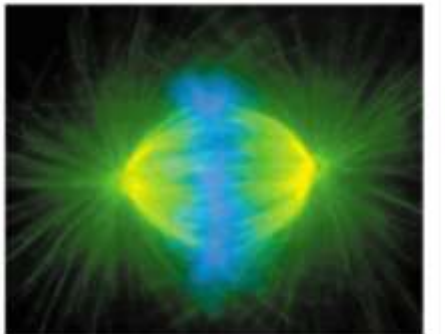

Release of $CO_2$(g) from saturated solutions of polymer and polymer + enzyme

**Reversible $CO_2$ capture is possible with the copolymer system!**

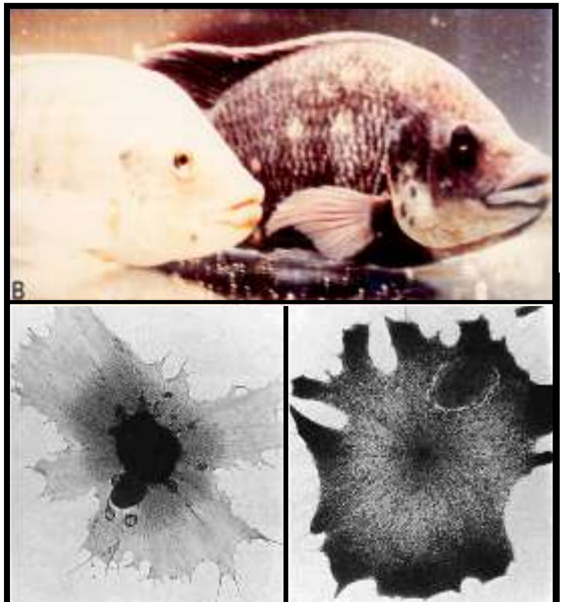
# Microtubule Mimicry: Biomolecular Self-Assembly in Synthetic

Sandia National Laboratories

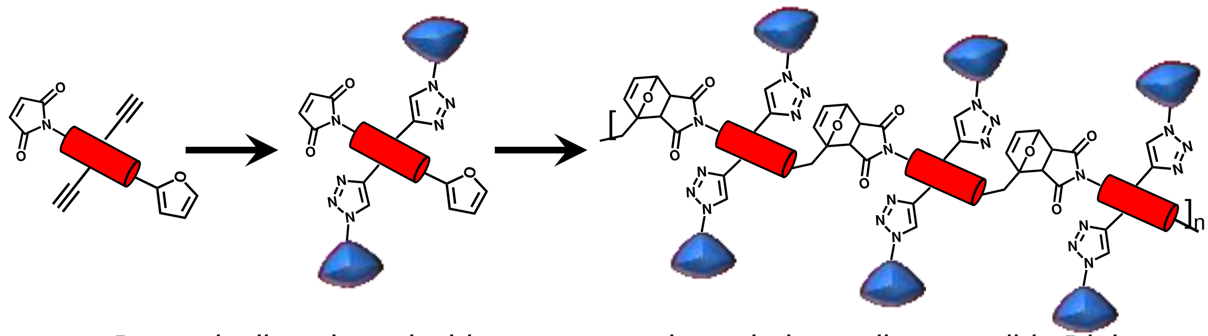
**_Program Goal: Utilize or mimic energy-consuming proteins in artificial systems for the active transport, assembly, and reconfiguration of nanomaterials._**



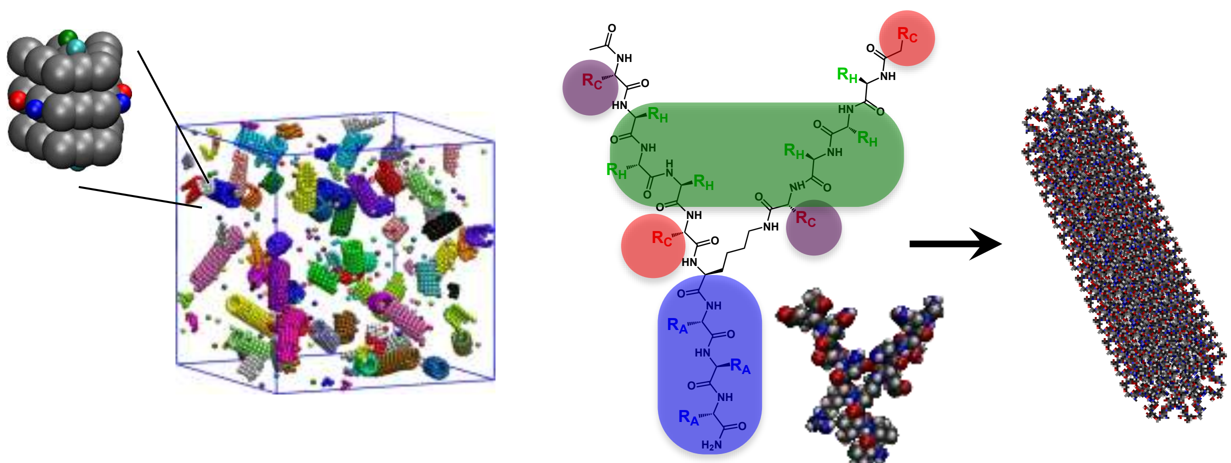
Chromosome positioning and separation during cell splitting



Adaptive reorganization of pigment granules in melanocytes



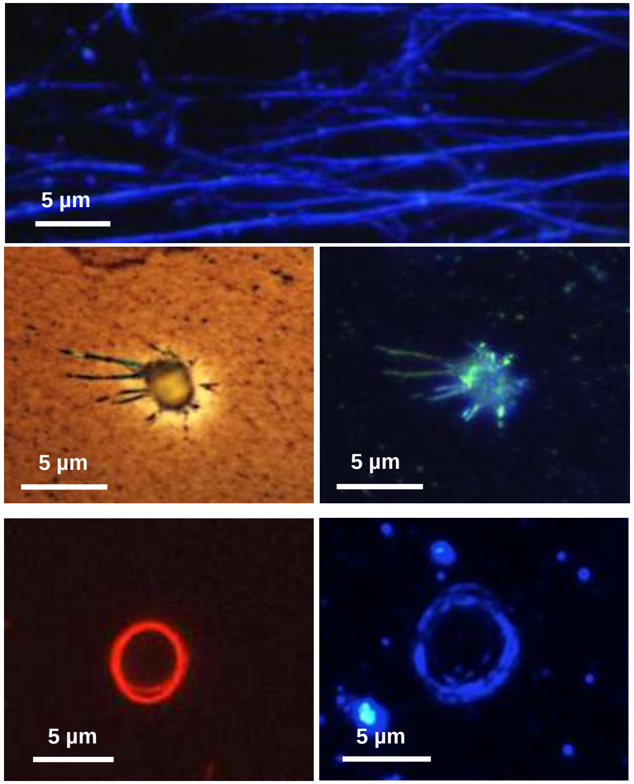
*Dynamically polymerizable monomers through thermally-reversible Diels-Alder chemistry.*

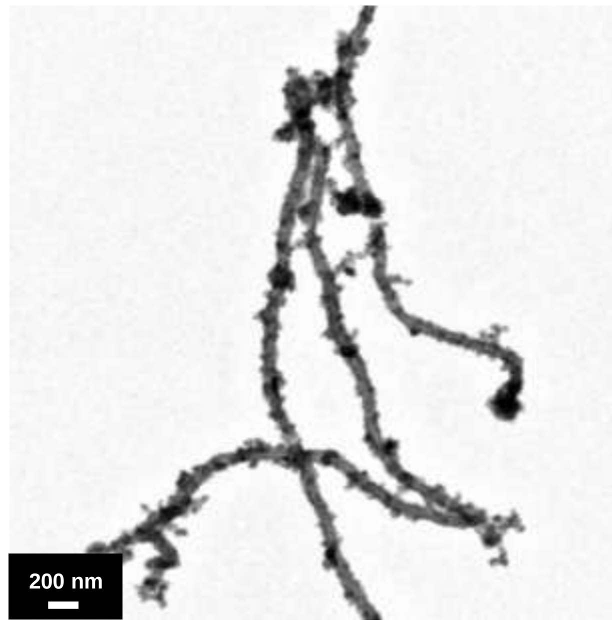


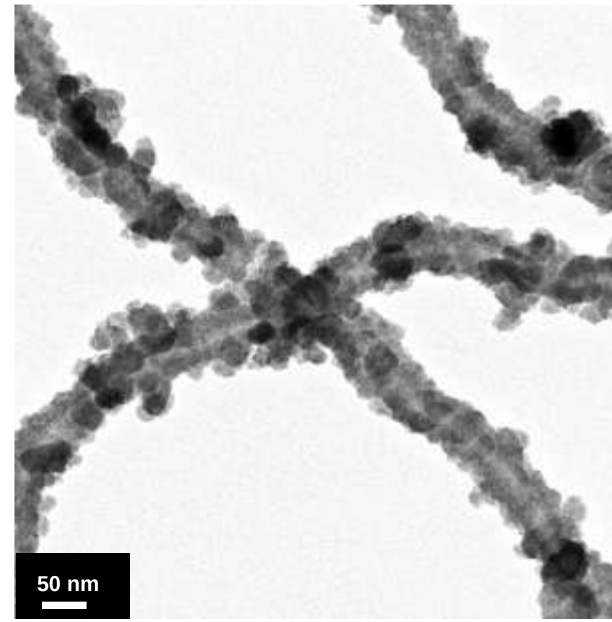
*Peptide Wedges provide a unique experimental platform for probing the effects of monomer design on assembly.*

# Microtubules: Templates for mineralization

CdS mineralized onto microtubule templates

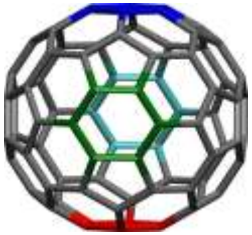
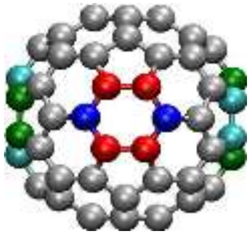
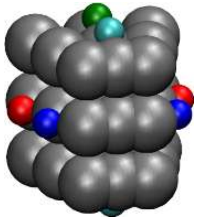
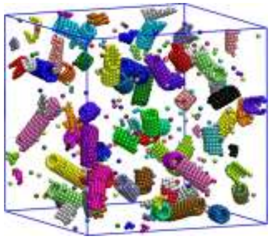



*Tubulin, the protein that assembled to form microtubules, contain amine, carboxyl, thiol, histidine and alcohol groups, which allow the fibers to nucleate and grow inorganic crystals.*

# Molecular Dynamics Establish Design Rules for Assembly

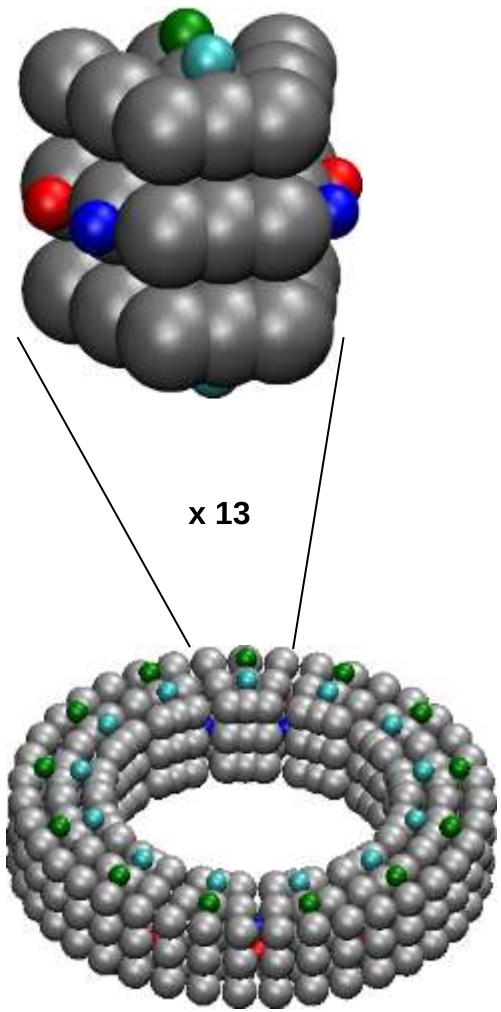
| | Monomer Building blocks | Polymerized Structures |
|---|---|---|
| Sphere with symmetric attractive sites |  |  |
| Sphere with broken symmetry |  |  |
| Wedge with broken symmetry |  |  |

**Assembly Parameters**

- Gray sites are repulsive
- Red:blue and green:cyan are attractive
- Like colored sites are repulsive

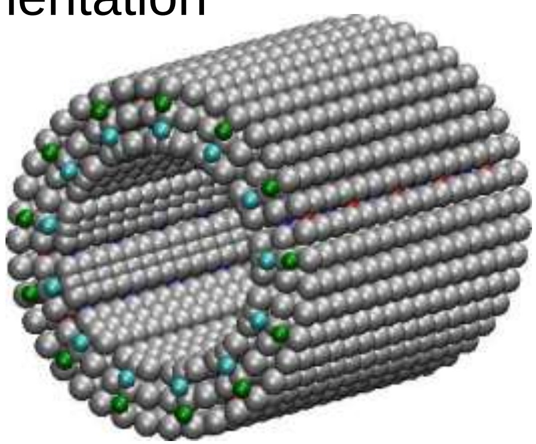
*Monomer shapes as well as strength and geometric distribution of interaction potentials on each monomer are critical*

# Asymmetric Wedge Building Blocks Form Tubular Structures

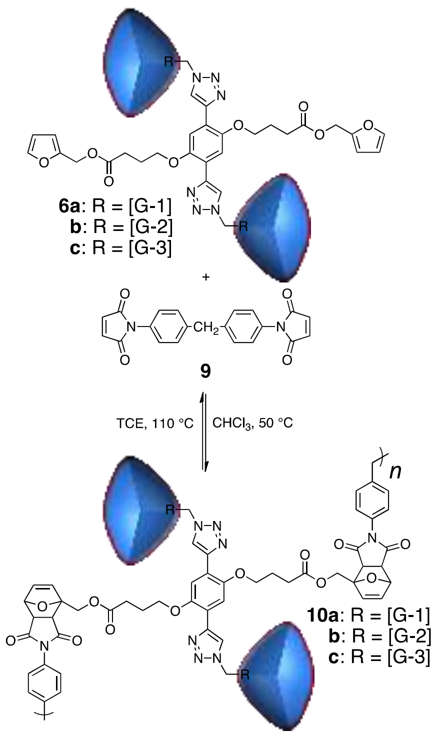



Wedge monomers with broken symmetry provide:

- Shape
- Lateral Interactions
- Vertical Interactions
- Molecular Orientation



# Reversible Thermal Assembly of Dendronized Polymers

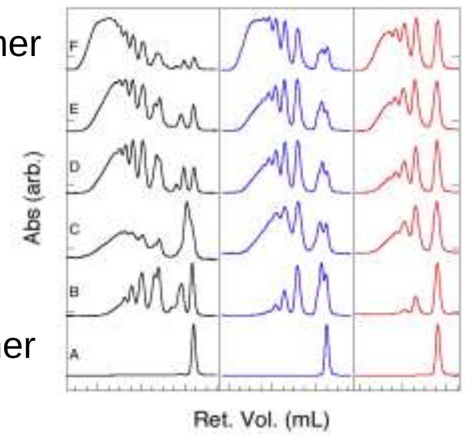



TCE = 1,1,2,2-Tetrachloroethane

Gel Permeation Chromatography

**Assembly**

Polymer

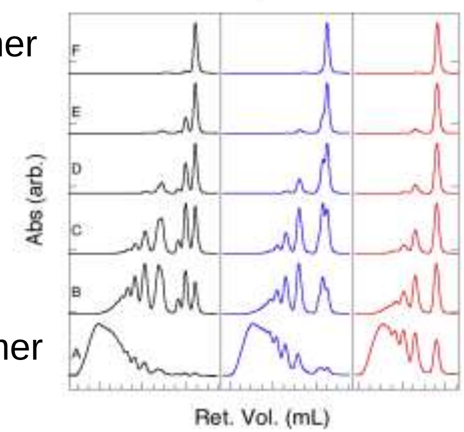



Monomer

288 hrs
120 hrs
48 hrs
24 hrs
8 hrs
$t_0$

**Disassembly**

Monomer




Polymer

40 min
30 min
20 min
10 min
5 min
$t_0$

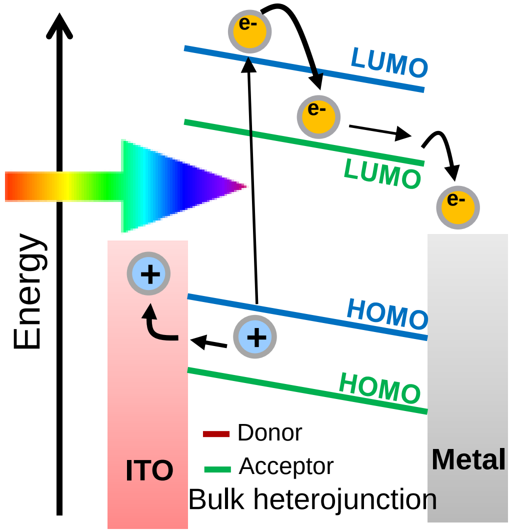
*Chromatography (GPC) shows the thermally reversible polymerization of dendritic building blocks.*

Macromolecules (2010)

# Nanocrystalline Framework Photovoltaics

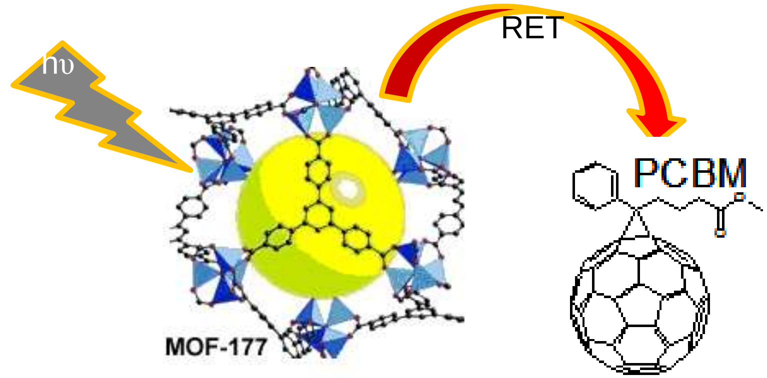
Sandia National Laboratories

***Goal: Explore the effect of nanostructure on PV performance***



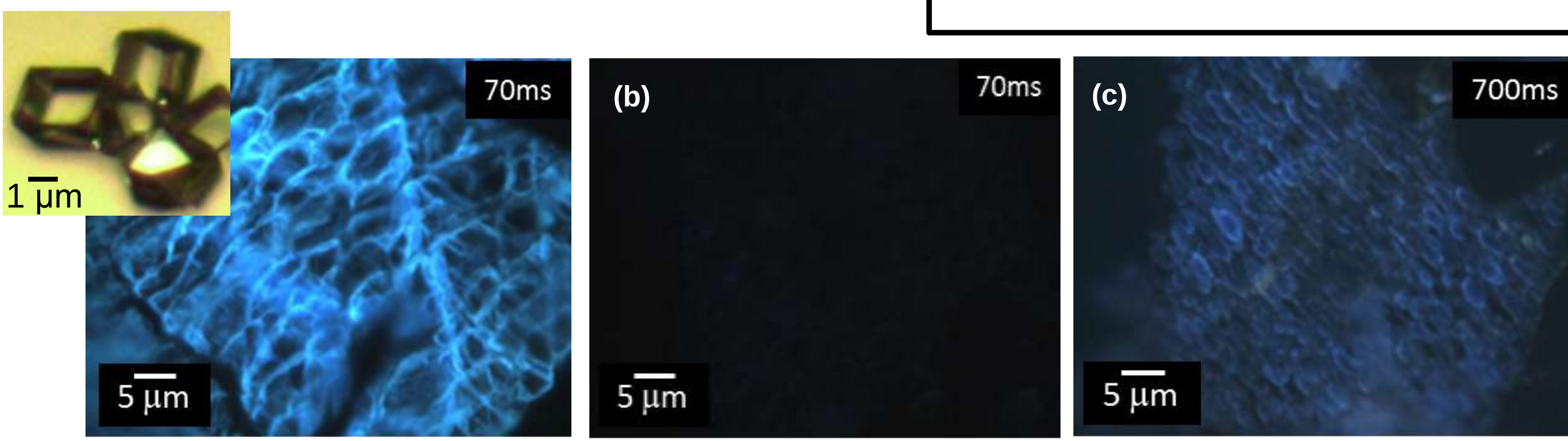

Light absorption excites electrons into donor CB.

Electrons then pass to the acceptor in order to get current from a device.




Nanostructured donor framework infilled with an acceptor.

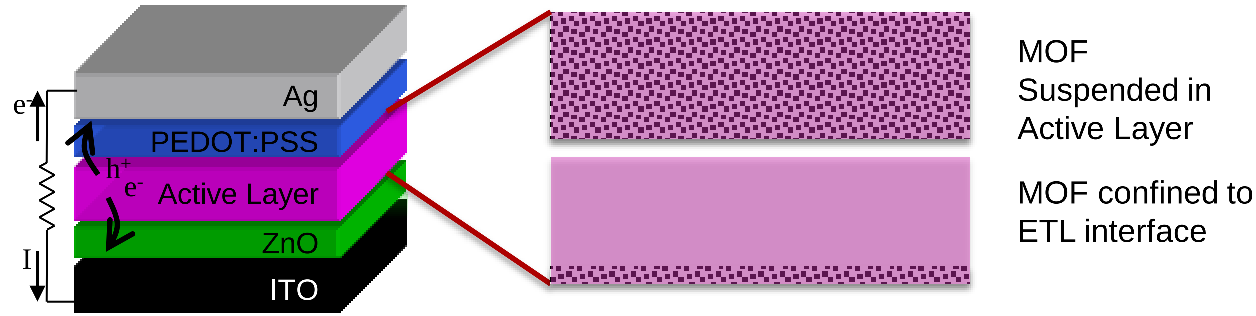
Electrons are excited in the framework and passed to the fullerene acceptor.




Micro-luminescent images of MOF-177 crystals embedded in acrylic resin. Microtomed sections from the interior of (a) MOF-177 and (b and c) exposed MOF-177-PCBM complex.

# MOF-based PV Devices: Informing improved processing and performance

We have developed several techniques for integration of CNFs into hybrid OPV devices.




**Key lessons moving forward:**

- Connectivity/communication between active components is critical (ETL, donors, acceptors, etc.)
- CNF size/morphology will strongly affect device performance
- Creating dense CNF films will be important, particularly for active CNF components
- Active CNFs are preferred over "passive" structures – everything you put into the device affects performance!