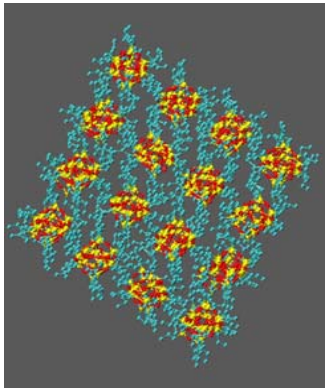
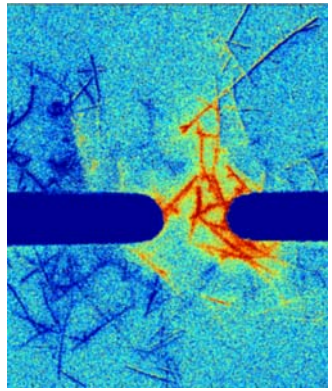




The Look Ahead: Center for Nanophase Materials Sciences

SNS-HFIR Users Meeting
October 11, 2005

Linda Horton
Director
Center for Nanophase Materials Sciences

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

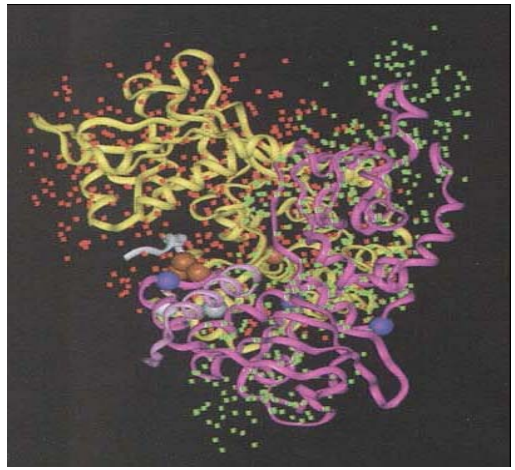
CNMS Oak Ridge National Laboratory Center for Nanophase Materials Sciences

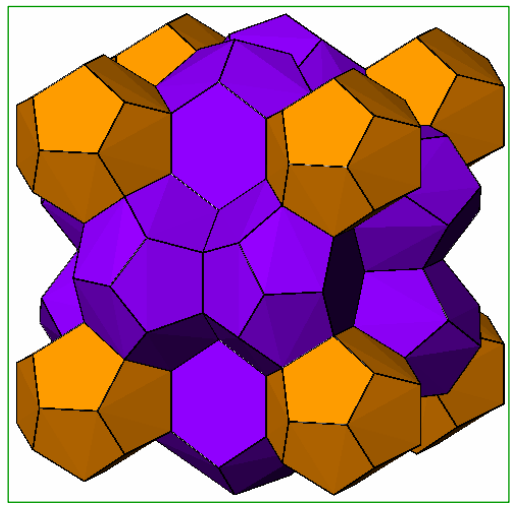
UT-BATTELLE

What is nanoscience

- A revolution in the way we look at the physical world
- Fills a gap between single atoms/molecules and larger microstructures
- Addresses materials behavior at dimensions of 1-100 nm
  - Properties depend on size
  - New and unexpected phenomena
  - Requires atom-by-atom assembly

Interactions of protein molecules





Natural methane storage in clathrate molecules

Why now?

- New tools for atomic-scale characterization
- New capabilities for single atom/molecule manipulation
- Computational access to large systems of atoms and long time scales
- Convergence of scientific-disciplines at the nanoscale

DOE's nanoscience centers

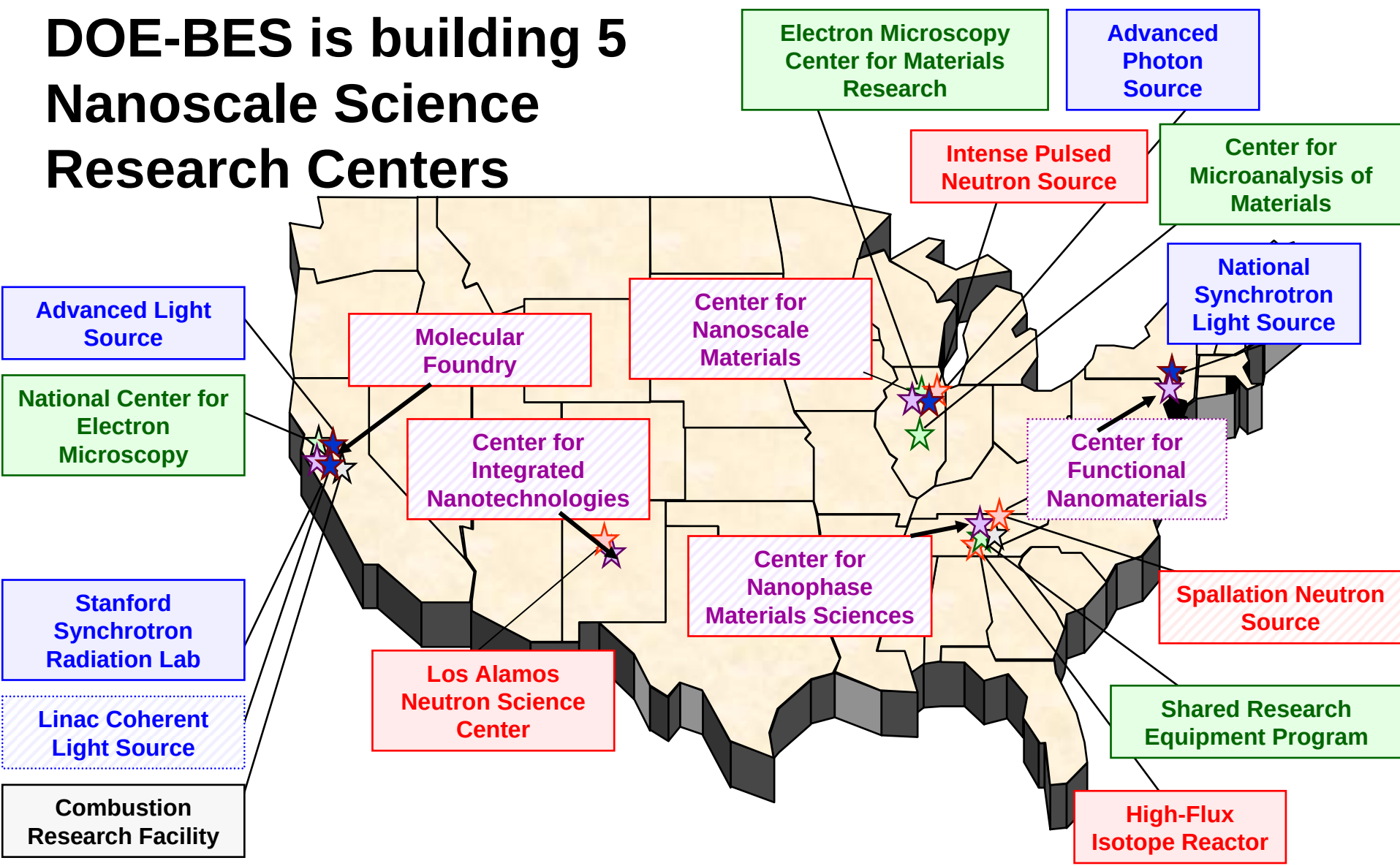
Neutron and synchrotron sources

Ultrascale computing

Center for Nanophase Materials Sciences: Background

- CNMS is one of five national user facilities being built by the Department of Energy
  - Began with a proposal competition in 2001
  - Supported by DOE's Office of Science, Office of Basic Energy Sciences
- The initial stage was the CNMS line item project to build a new facility: $65M
  - Substantial input from the technical community: workshops!
  - Included both the building and initial capital equipment
- There was an interim "jump start" user program funded by DOE-BES in 2004 and 2005
- First operations funding for the new facility is in FY06: $18.1M for both operations and capital equipment
  - Goal for FY06: 100 users
  - Longer term goal: 250 users per year

DOE-BES is building 5 Nanoscale Science Research Centers



Under construction

- *4 Synchrotron Radiation Light Sources*
- *Linac Coherent Light Source (CD0 approved)*
- *4 High-Flux Neutron Sources (SNS under construction)*
- *4 Electron Beam Microcharacterization Centers*
- *Special Purpose Centers*
- *5 Nanoscale Science Research Centers*

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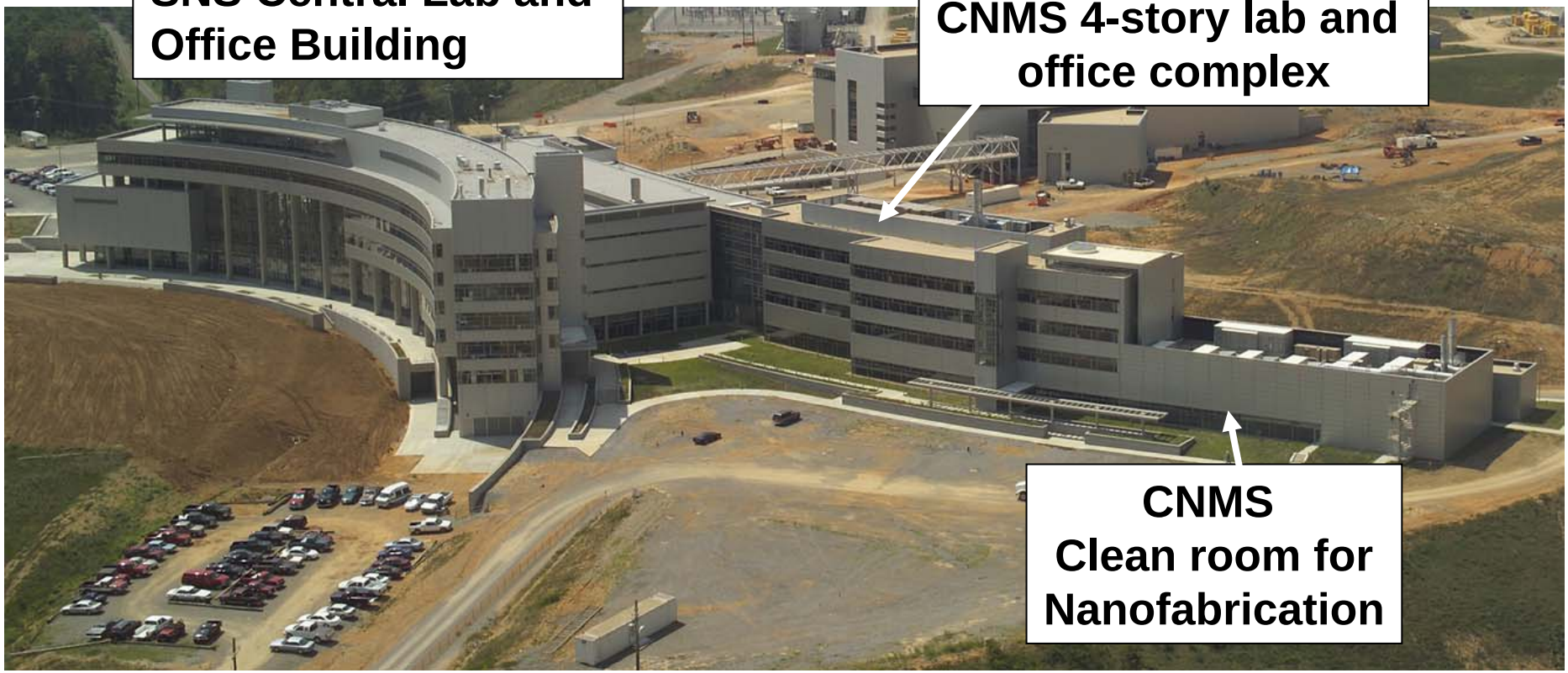
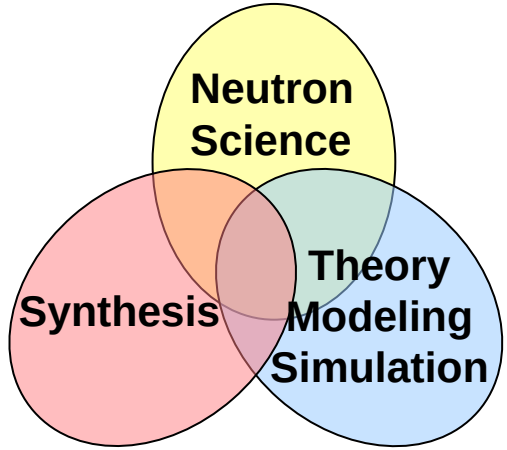
Center for Nanophase Materials Sciences: A National User Facility co-located with the Spallation Neutron Source



CNMS Conventional Facility
Construction: Completed - 80,000 sq ft

CNMS Integrates Nanoscale Science with 3 Synergistic Research Needs

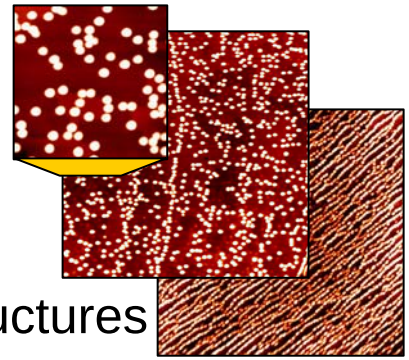


- Neutron Science
  - Opportunity for world leadership using unique capabilities of neutron scattering
- Synthesis Science
  - *Science-driven* synthesis: synthesis as enabler; evolution of synthesis via theory, modeling, and simulation
- Theory / Modeling / Simulation
  - Stimulate U.S. leadership in using theory, modeling and simulation to design new nanomaterials
  - Investigate new pathways for materials synthesis

CNMS Scientific Themes

Macromolecular Complex Systems
- Synthetic (polymeric) and bio-inspired materials

Functional Nanomaterials
- Nano- tubes, wires, dots, composites; artificial oxide film structures



AFM images of Fe nanodots and nanowires on flat and stepped NaCl surfaces (edge length 750 nanometers)

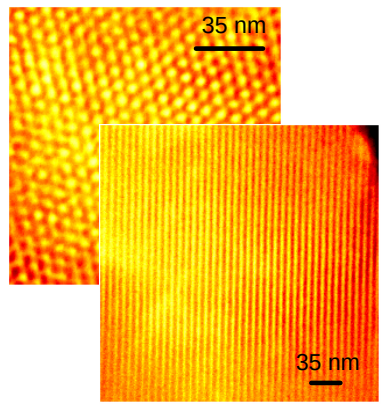
Nanoscale Magnetism and Transport
- Reduced and variable dimensionality; quantum transport

Catalysis and Nano-Building Blocks
- Highly selective catalysts; nanoscale synthesis & organization

Nanomaterials Theory Institute: Theory, Modeling, Simulation
- Grand challenges of “computational nanoscience”

Nanofabrication Research Laboratory
- Controlled synthesis & directed assembly; functional integration of “soft” and “hard” materials

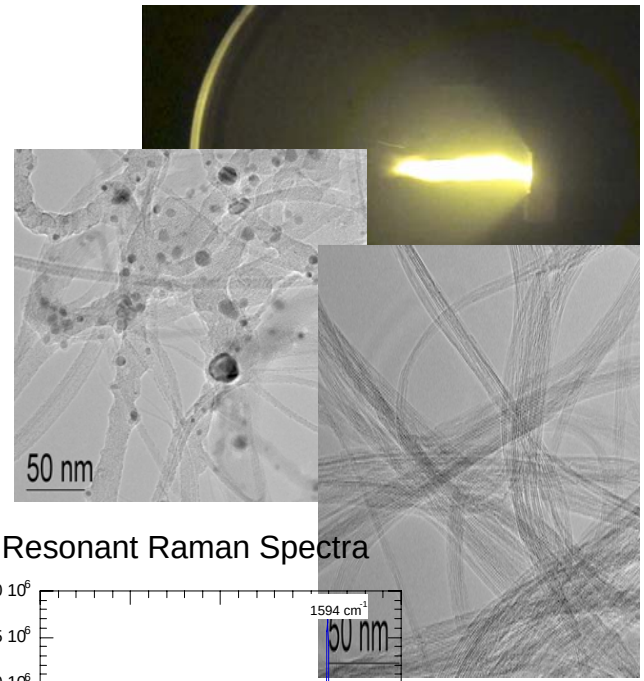
Nanoscale Imaging, Characterization, and Manipulation
- Unique instruments to characterize and manipulate nanostructures; simultaneous imaging and environmental control



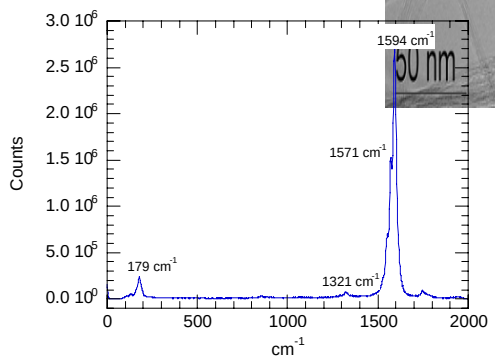
Ordered nanoporous silica synthesized using an organic template

Each Floor of the CNMS has a Technical Focus

- Ground Floor: Clean room and sensitive instrumentation, including microscopes and scanning probes
- Level 1: Laser labs and other heavy equipment; administration and user administrative support
- Level 2: Catalysis, soft material characterization, and CVD laboratories; theory office and workstation/server room; interaction space lit by a sky light
- Level 3: Wet chemistry laboratories for macromolecular and carbon materials, catalysis; theory offices



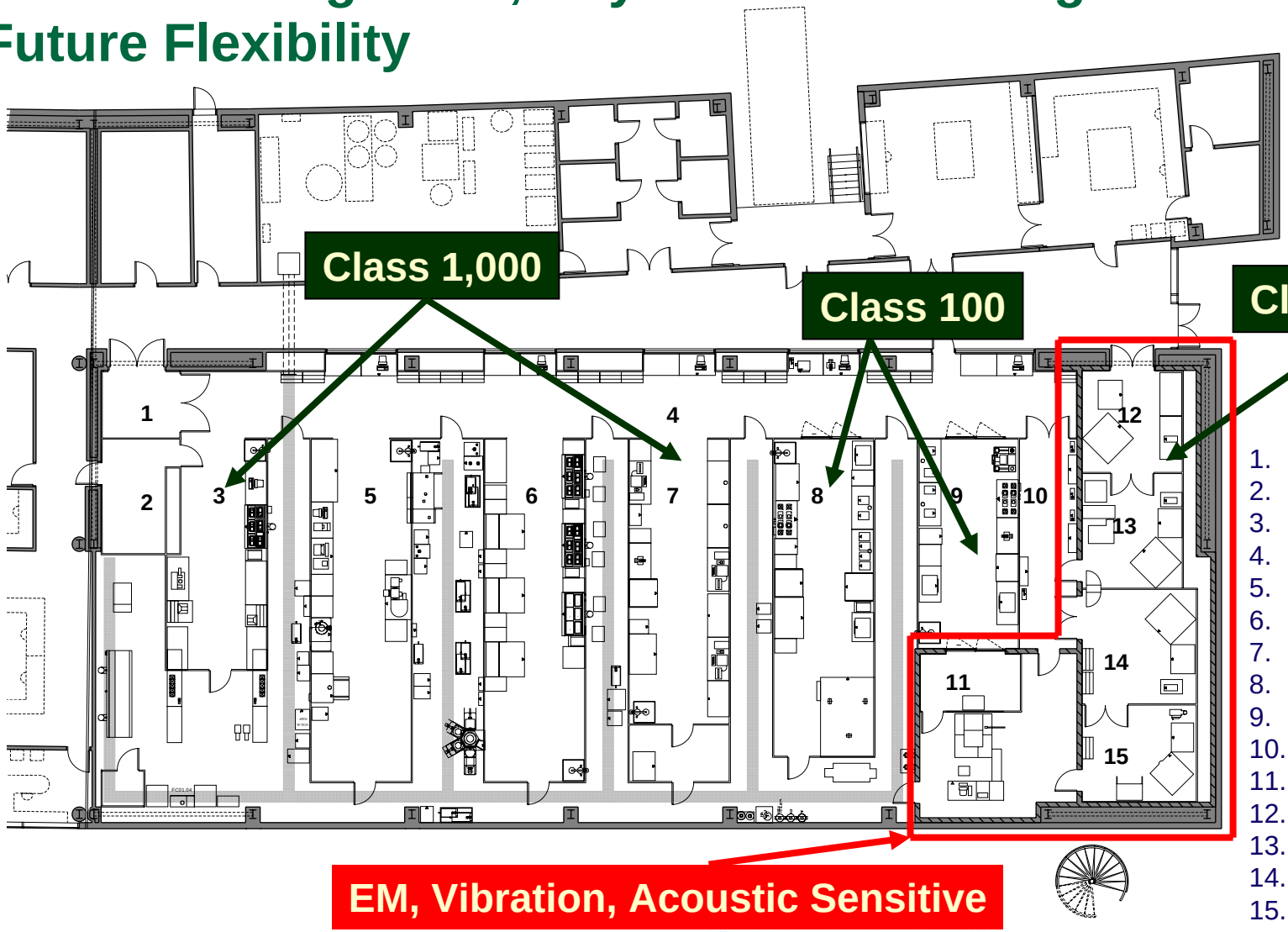
Resonant Raman Spectra



Each floor has similar layout: labs across from offices; central interaction space and conference rooms; additional interaction space on upper floor bridges

Ground Floor: Clean room and sensitive instrumentation, including microscopes and scanning probes

CNMS Clean Room – Important for Directed Assembly and Materials Integration; Bay and Chase Design Allows for Future Flexibility



Direct Write Electron Beam Lithography (DWEBL) System

- **Scientific Driver: Nanofabrication**
  - **Patterns of arbitrary shape and size, with dimensions as small as 5 nm, can be fabricated on essentially any flat substrate that is sensitive to electron irradiation or is coated with electron beam resist.**
- **Capabilities**
  - **100 keV thermal field emission source**
  - **Substrate handling capabilities for small pieces, membrane structures and whole substrates up to 8–inch diameter**
  - **Laser interferometer with sub–nanometer resolution to permit highly accurate mechanical positioning**
  - **Substrate–height sensor to permit dynamic corrections to the beam focus**
- **Cost: $4.9 M**
- **Vendor: JEOL**

CNMS e-beam at JEOL in December
Factory Acceptance Tests: Successful!
Installation nearly completed

Synthesis Laboratories: Hoods!!

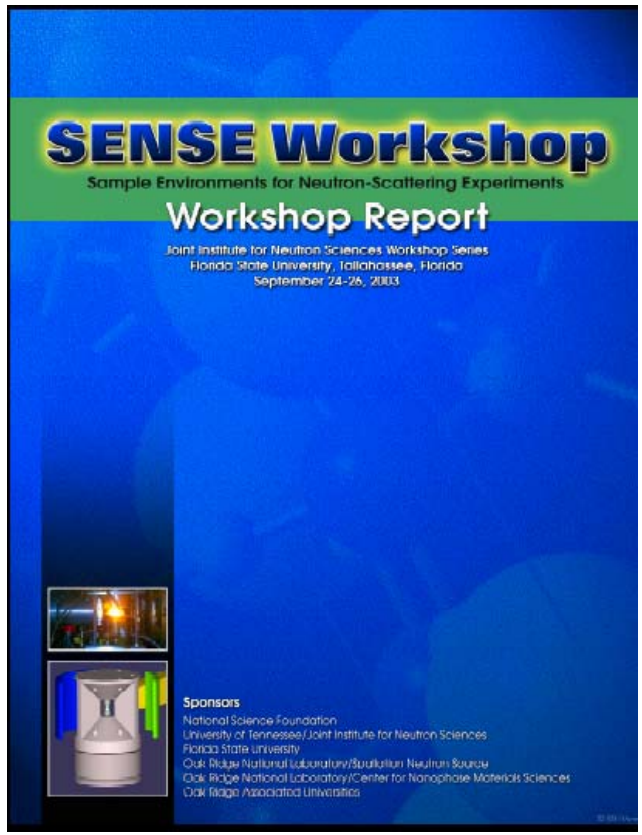
Hoods!
3 – 10’ Walk-in
6 – 8’ Walk-in
24 – 8’ Bench
3 – 6’ Bench
5 canopy hoods
1 laminar flow

Unique and State-of-the-Art Capabilities in Macromolecular Science

- **"One-stop-shopping" for all polymer needs**
  - **Synthesis, characterization, deuteration**
- **State-of-the-art synthetic techniques to prepare complex polymer architectures**
  - **Stars, combs, hyperbranched polymers**
  - **Available in only a few labs world-wide**
- **Unique new capabilities to prepare and characterize polymer-carbon nanotube composites**
  - **Currently available to users in "jump start"**
- **Emerging synthetic capabilities to prepare novel polymer architectures**
  - **Based solely or partially on amino acids**

Need for Deuterated Materials

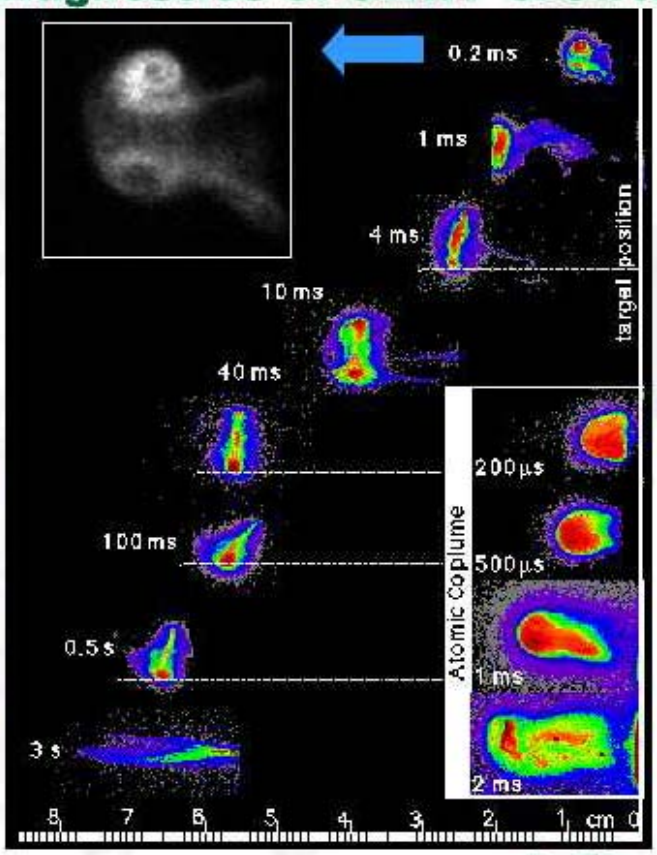
- NSF Workshop on Neutron Scattering for Chemistry and Chemistry/ Biology Interface, and NSF Workshop on Sample Environments for Neutron Scattering Experiments, September 23-26, 2003
  - "Providing users with the tools and facilities needed to produce deuterated materials would enhance both the quality and quantity of neutron experiments that can be done at SNS and other neutron research centers, and would make feasible new and more sophisticated experiments than can be presently performed."
- Recommendations:
  - "A top priority (is)…sample preparation laboratories, including deuteration facilities, convenient to the beam line."
  - "Create a general deuteration/isotope materials facility for the production of deuterated and novel isotopically substituted materials..."
  - "Develop methods for the synthesis of labeled polymers, peptides, surfactants, and other complex biomolecules and other small molecules of interest."
- CNMS is uniquely posed to address many of the deuteration needs of the scientific community

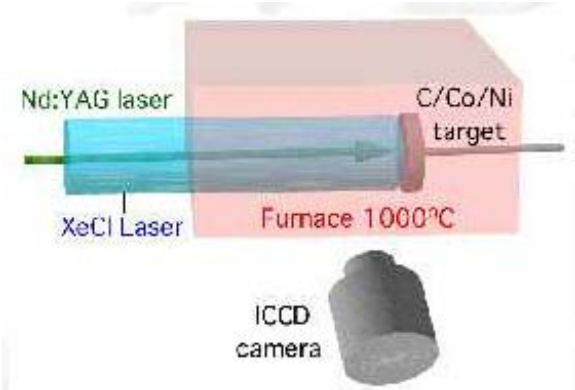


Vision for Outstanding Science

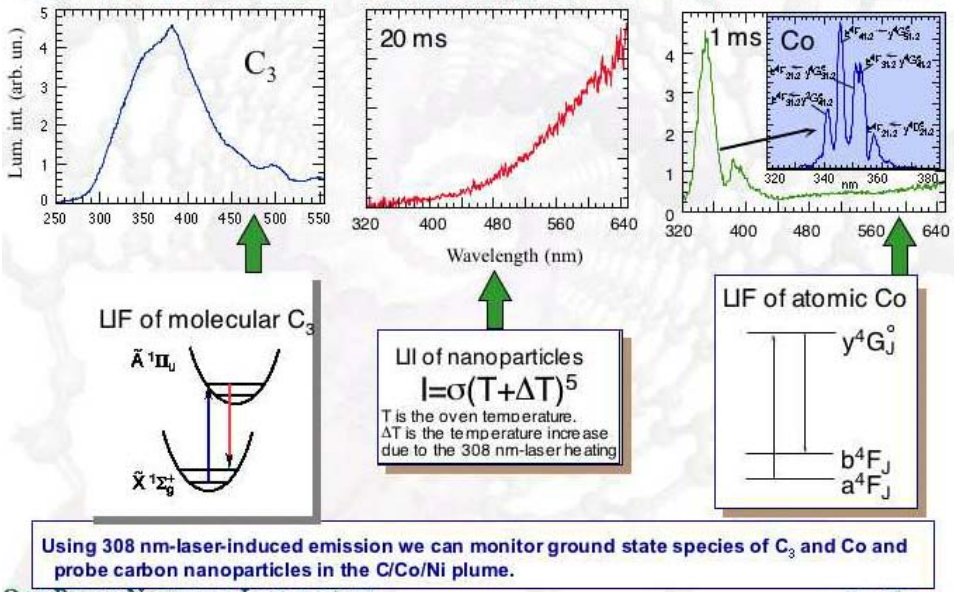
In situ Spectroscopic Diagnostics of Nanomaterials Growth

Imaging and Spectroscopy Diagnostics of SWNT Growth





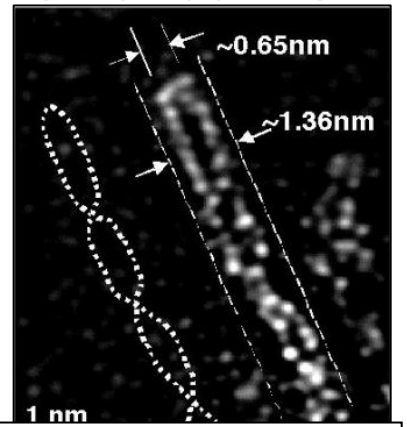
Laser-Induced Emission Spectra of C/Co/Ni Plume at 1000° C During Nanotube Growth



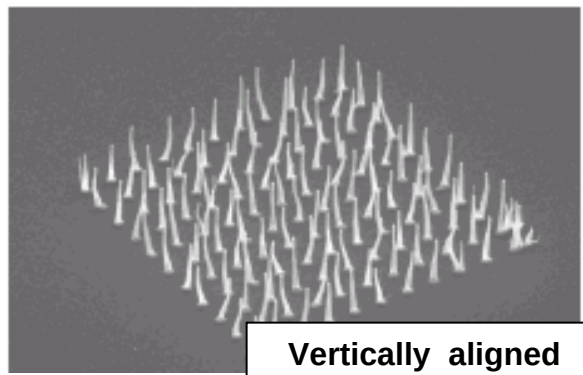
Nanoscale Imaging, Characterization and Manipulation

New techniques and instruments for imaging, characterization and manipulation of soft and hard materials, with environmental control

- Neutron and X-ray Scattering
  - Specialized scattering techniques and environments for nanoscience
- UHV Scanning Probes
  - UHV scanning probe microscopies for magnetic and quantum transport properties in nanostructured materials
- Electron Microscopy and Spectroscopy
  - Combine imaging with characterization and/or manipulation methods
  - Special sample environments (soft materials); in situ spectroscopy; integrated use of ambient scanning probes

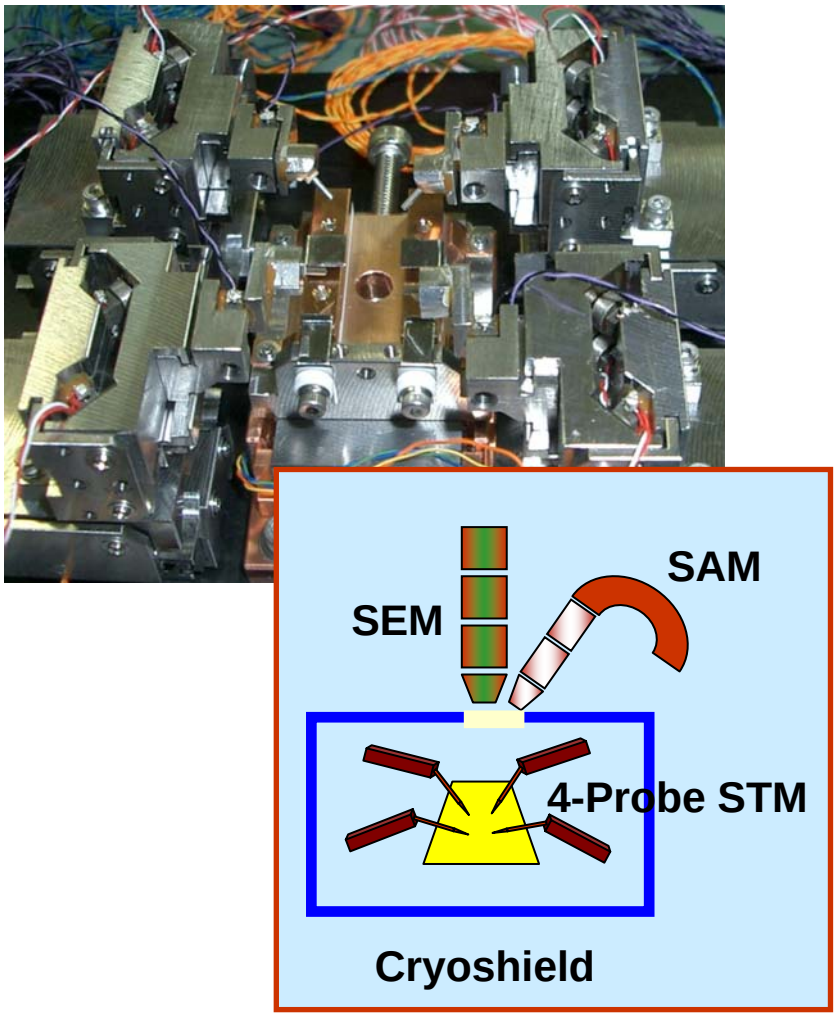


Single-walled carbon nanotube containing helical chain of iodine atoms



Vertically aligned carbon nanofibers

Four-point Probe STM with SEM:
Manipulation & Transport in Nanoscale Systems

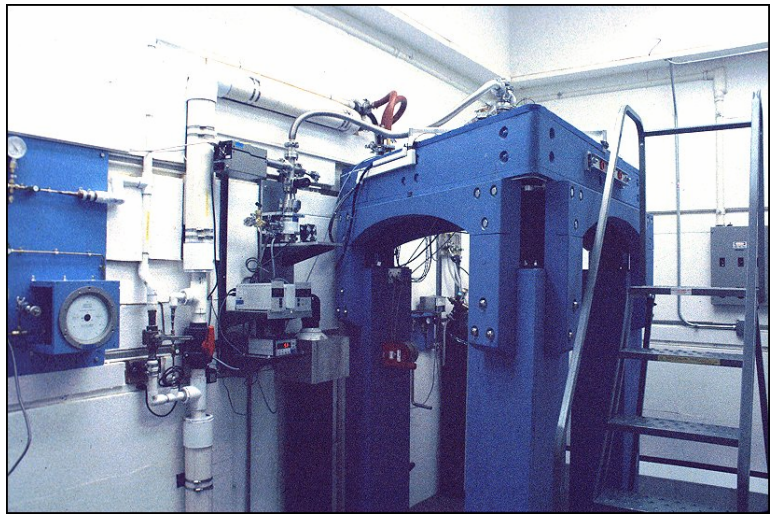


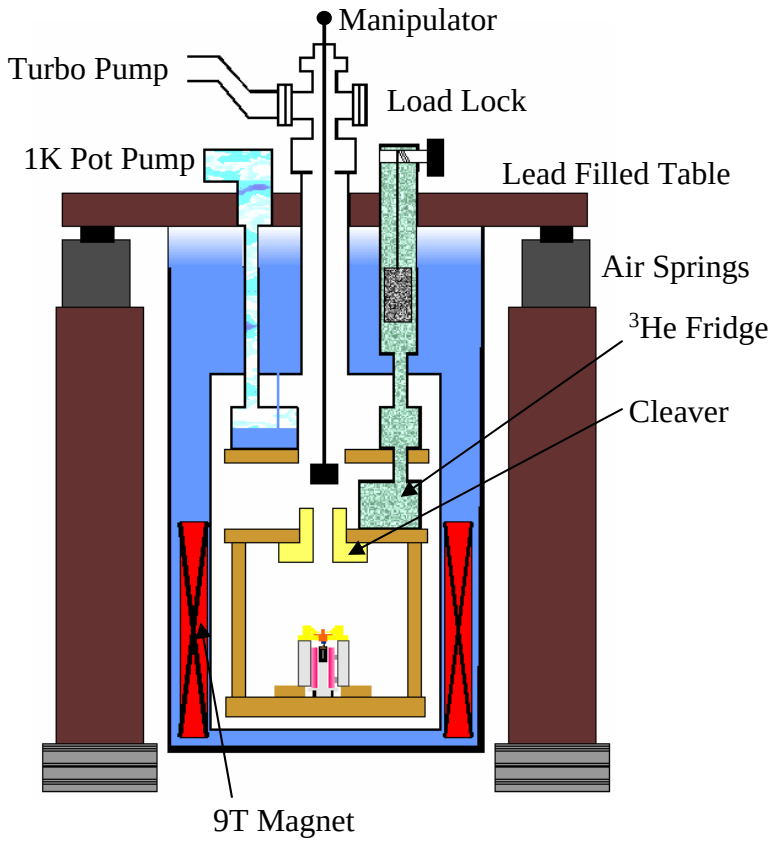
- **Scientific Drivers**
  - Temperature-dependent quantum electrical transport of nanoscale objects on surfaces
  - Manipulation of individual nano-objects
  - Fabrication and characterization of nanoscale devices
  - Spintronics / spin injection / spin transport
- **Capabilities**
  - Four probes operate independently, tip separation < 100 nm
  - Integrated SEM with resolution < 10 nm permits accurate positioning of four tips relative to each other and to nanofeatures of interest
  - 20 K < T < 600 K
  - UHV-capable (5 x 10^{-11} Torr)
  - Integrated sample preparation / handling
  - Scanning Auger Microscope (SAM) allows elemental identification of nanostructures
  - Nanofabrication: STM tip-stimulated chemical vapor deposition (CVD)

The “Ultimate STM”

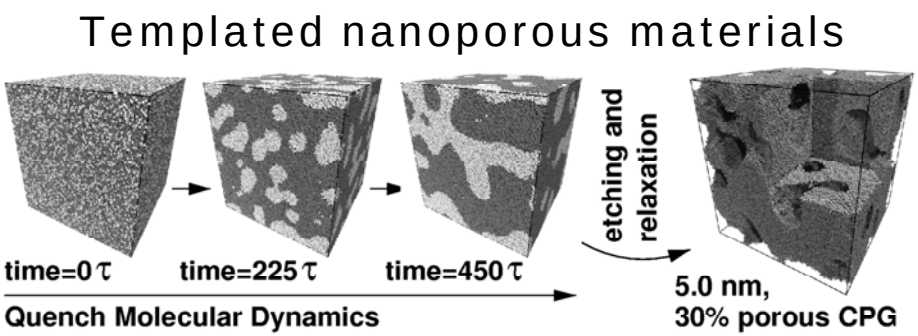
- Single-atom or -molecule spectroscopy
- Atomically-resolved spectroscopy maps
  (Requires vertical resolution of <0.0001 nm, ~100X better than commercial instruments.)
- k-space mapping of electronic structure
- The temperature and magnetic field range to study the quantum response of nano-objects
- Optical access to the sample in magnetic field, for probing and exciting atoms or molecules
- Sample rotation (STM) in the magnetic field
- Flexibility to convert this STM to a magnetic scanning microscope with atomic resolution
- Joint development: ORNL, Univ of TN, Univ of Texas

- 300mK < T < 150K
- B_{max} ~ 9.0 Tesla
- Sample exchange from RT
- Cryogenic UHV Sample Cleavage





Theory, Modeling and Simulation: A Core CNMS activity



- Develop **accurate** new theoretical tools with **predictive** capabilities
- Synthesize materials with **designed-in** new combinations of properties
  - **Multi-Scale Modeling:** Link atomic-, nano-, and micro-scale structures and calculate properties up to the macroscale
  - **Nanomaterials Design:** New structures for new properties
  - **Virtual Synthesis:** Theoretically evaluate & predict new growth pathways
  - Provide **access** to **world-class computational facilities and expertise: ORNL's Center for Computational Sciences coupled with CNMS research staff, postdoctoral scholars, visitors**
    - **25 teraflops in FY05; 100 teraflops planned for FY06**
  - **CNMS 80-dual processor node Beowulf Cluster**
    - **4 GB RAM per node; gigabit interconnects; 1.1 teraflop**
  - **Bring together world leaders** in theory / modeling / simulation

Jump Start Nanoscience Research: Enthusiastic Response to FY04 and FY05 Calls for Proposals

~135 PROPOSALS RECEIVED

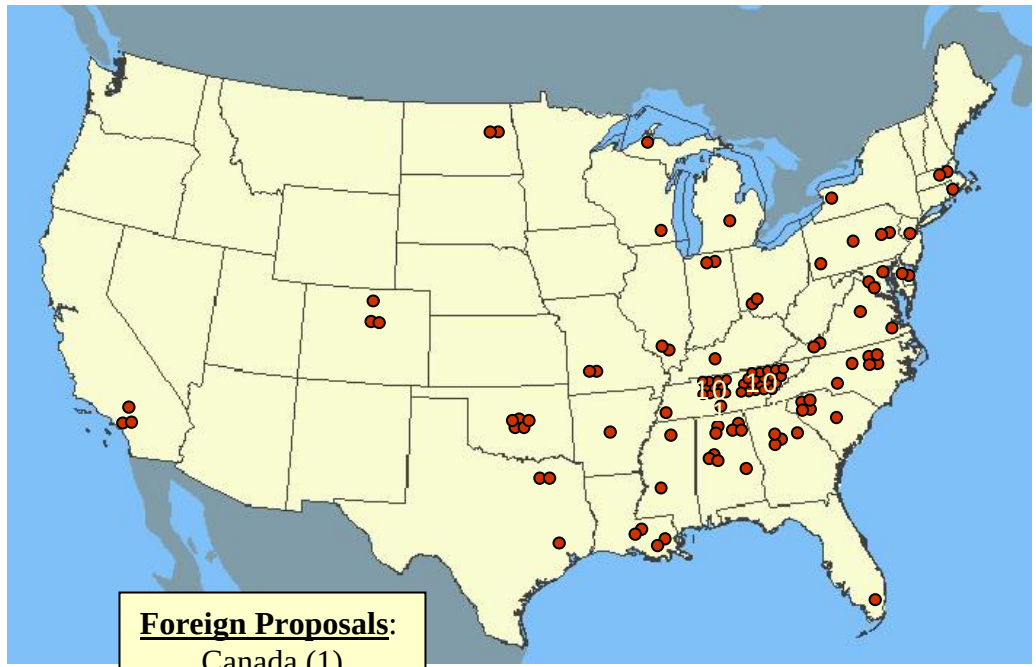
- **24 states represented**

DISTRIBUTION BY SOURCE

- **96 universities**
- **8 industry**
- **5 Other DOE and Federal Laboratories**
- **19 ORNL**
  - **Some with university collaborators**
- **7 foreign**
  - **Germany, France, China**
- **FY04: 41 proposals selected based on external *peer* review**
  - **~ 10 on proof-of-concept basis**
- **FY05: 32 proposals selected**
- **All active user research proposals listed on CNMS web site**

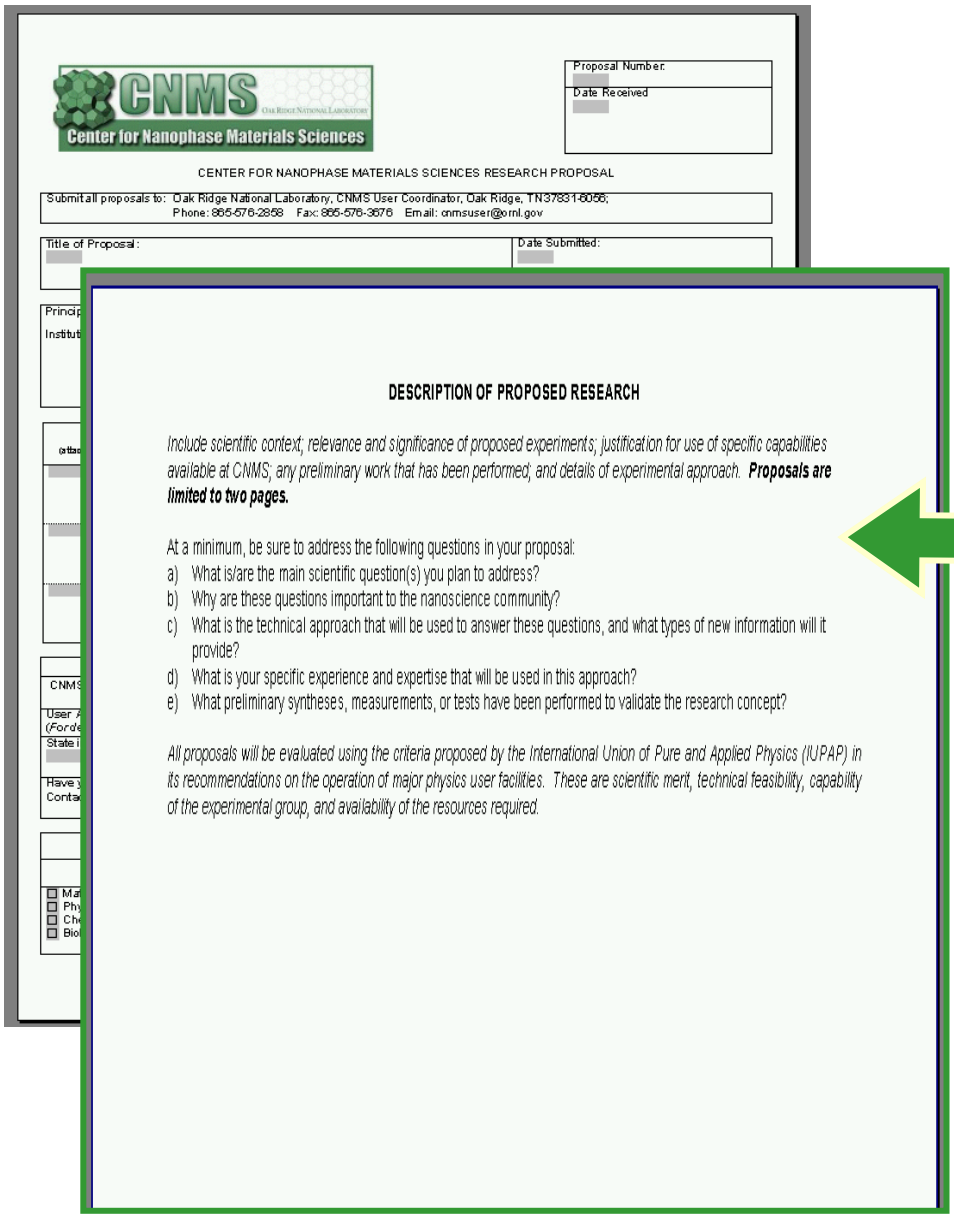
First Full-Scale Call for Proposals for FY06

- About 120 new proposals
  - Projection: Accept 50
- Second FY06 Call for Proposals planned for January-February 2006
  - Goal: 100 total new proposals accepted for FY06



Foreign Proposals:
Canada (1)
China (3)
Italy (1)
Mexico (2)
Taiwan (1)

User Program and Call for Proposals



- **Proposals accepted on a specified schedule:**
  - **Steady state 2 - 4 cycles/year**
  - **Next call Jan-Feb 2006**
- **Features:**
  - **Equipment checklist**
  - **ES&H checklist**
  - **Two-page project description**
- **Internal review for feasibility**
- **Peer-reviewed by entirely external Proposal Review Committee, with experts in each research area**
- **Coordinated with other User Facilities at ORNL**

CNMS is a Research Partner with the SNS and HFIR

- **CNMS has unique synthesis tools and characterization tools that complement neutron scattering**
  - "One-stop access" for synthesis, characterization, and theory facilities and expertise
- **A dynamic environment to catalyze revolutionary approaches and train the next generation of researchers**
- **Development of next-generation techniques, instrumentation, and codes that benefit a broader technical community**
- **Integration of the user communities**
  - **Single proposal, good coordination, ease of proof-of-principle experiments**

Advantages of Co-location

- "One-stop access" for synthesis, characterization, and theory facilities and expertise
- A dynamic environment to catalyze revolutionary approaches and train the next generation of researchers
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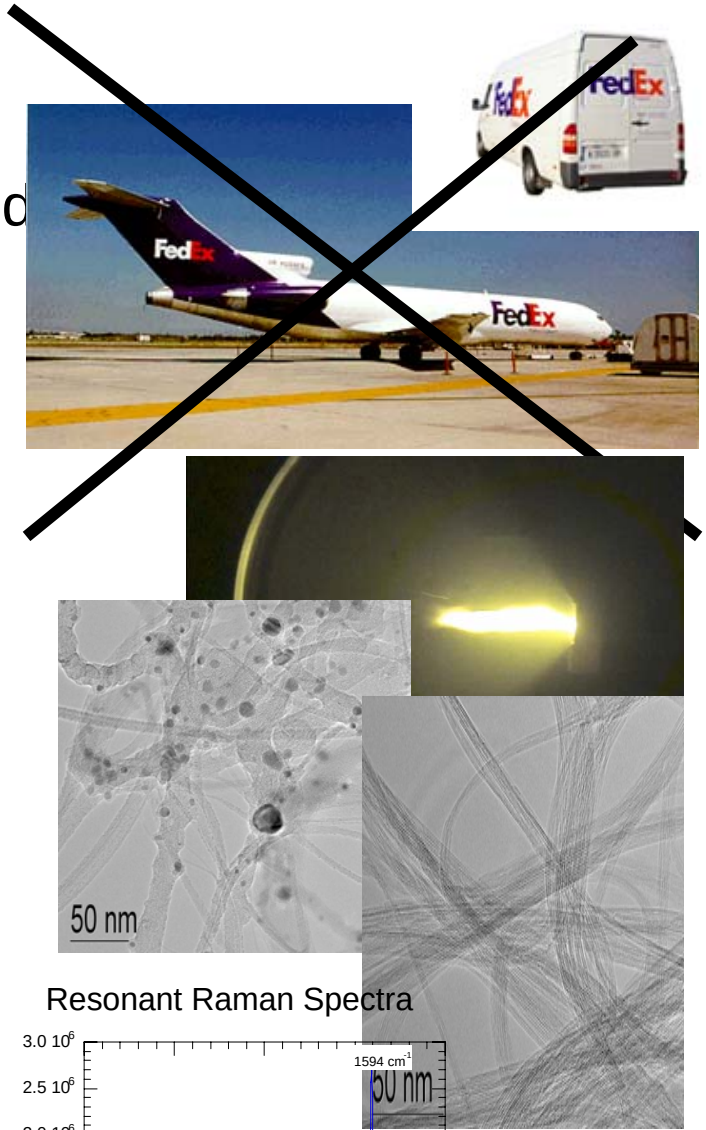
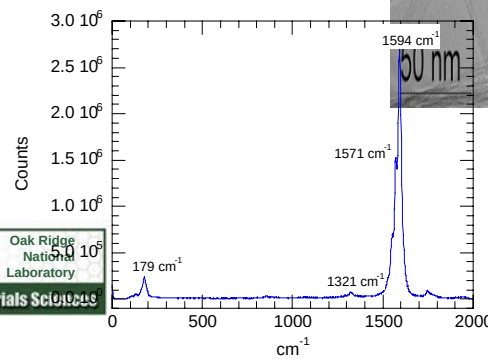
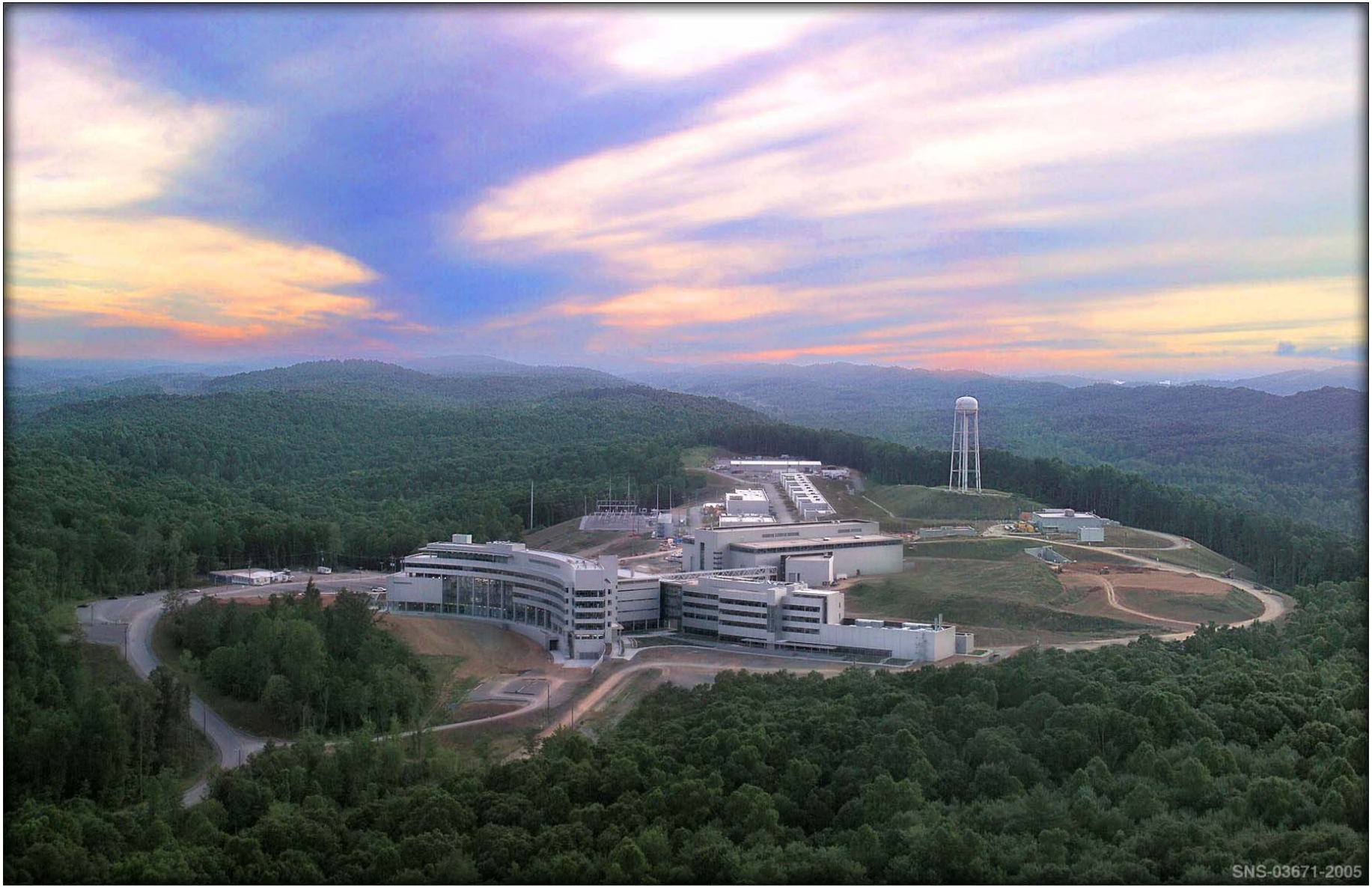


Resonant Raman Spectra




SNS-03671-2005

www.cnms.ornl.gov

Users will Benefit from Co-location of Capabilities at ORNL

- **Advanced Synthesis and Characterization Expertise**
- **Neutron Scattering**
  - In-situ phenomena
    - special environments synthesis, processing, evolution in environment
  - Magnetic properties, Dynamics
  - Soft Materials, especially with H/D substitution
- **Leadership Computing**
  - Theory and modeling are critical to advances in nanoscale research
    - Capability computing: Nanoscience end station requires both nano and computational expertise
  - Analysis and visualization of large data sets (including neutron scattering)
- **Microscopy**
  - A natural partner in nanoscale research
  - TEAM focus on next generation microscopy