



# Center for Nanophase Materials Sciences

*A Highly Collaborative and Multidisciplinary  
U.S. DOE Nanoscale Science Research Center*

CNMS HOME

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RESEARCH

BECOMING A USER

WORKING AT CNMS

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NEWS/HIGHLIGHTS

UPCOMING EVENTS

PEOPLE

CNMS POSTDOCS  
AND FELLOWSHIPS

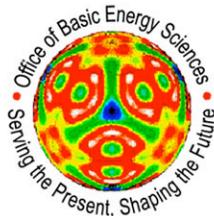
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CONSTRUCTION  
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SCIENCES



## **Scientific Themes, User Program, and FY03 "Jump Start"**



**Doug Lowndes**  
Scientific Director, CNMS

**DOE Nanoscale Science Research  
Centers Workshop**

**1<sup>st</sup> National Users Meeting**

Washington, DC  
February 28, 2003

# ***The Center for Nanophase Materials Sciences***



- A ***highly collaborative*** and ***multidisciplinary*** nanoscale science user research and research education center
- ***Developed in partnership with the university community***

OAK RIDGE NATIONAL LABORATORY  
U. S. DEPARTMENT OF ENERGY



1<sup>st</sup> NSRC User Workshop



## ***Scientific Scope and Vision***

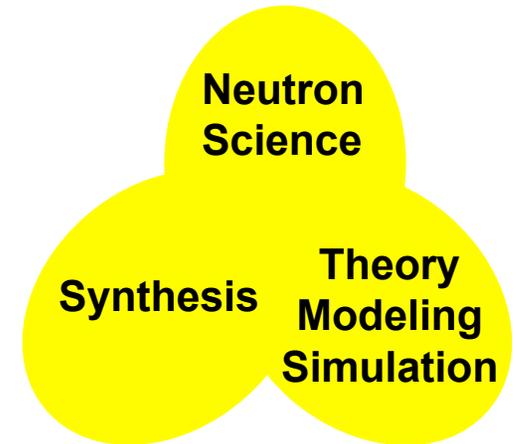
# **Center for Nanophase Materials Sciences**

- **Co-located** with the **Spallation Neutron Source (SNS)** and the **Joint Institute for Neutron Sciences (JINS)** on ORNL's "new campus"
- **JINS:** Housing and dining facilities, auditorium, classrooms, for research visitors and students
- **SNS:** Provides access to unique neutron scattering capabilities for nanoscience
- **CNMS:** Provides urgently needed capabilities for materials synthesis and characterization, nanofabrication, theory and modeling, and design



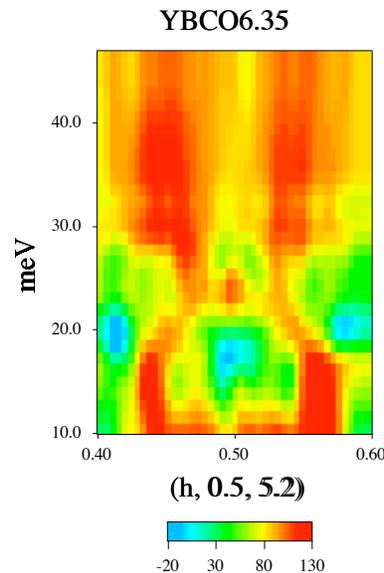
***The CNMS Concept:  
Create scientific synergies  
to accelerate discovery in nanoscale science***

# CNMS Integrates Nanoscale Science with 3 Synergistic National Research Needs



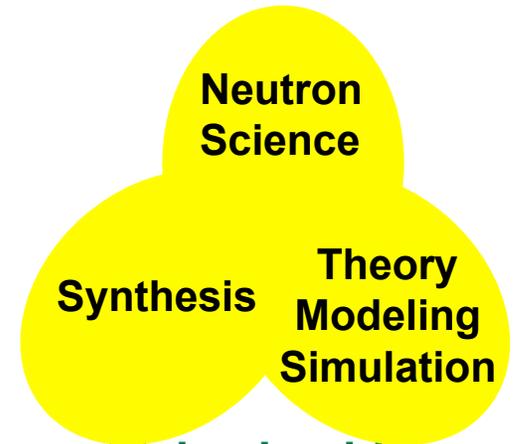
- **Neutron Science** [ SNS + Upgraded HFIR ]

- Challenging nanoscience focus: Opportunity for **world leadership** using neutron scattering to understand nano-materials & processes
- CNMS will exploit neutron scattering's **unique** and **complementary capabilities** to probe **soft** and **magnetic** materials & phenomena



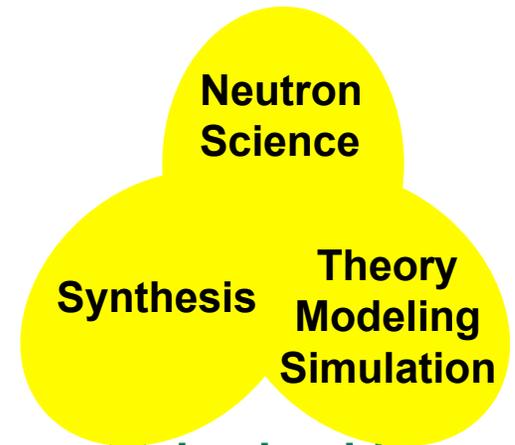
*Measurements of the magnetic scattering in YBCO high-temperature superconductors reveal the structure resulting from a nanoscale-to-mesoscale striped phase*

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- **Synthesis Science [ Nanofabrication Research Lab, NRL ]**
  - **Science-driven** synthesis: Key role of synthesis as **enabler** of new generations of advanced materials; **evolution** of synthesis via TMS
  - More efficient Search & Discovery methods; new synthesis pathways
  - NRL enables: **Controlled** synthesis and **directed** assembly of functional nanomaterials; **integration** of “soft” and “hard” materials

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- **Theory / Modeling / Simulation (TMS) [Nanomaterials Theory Institute]**
  - Stimulate U.S. leadership in developing new **nanomaterials design** and **virtual synthesis** tools
  - Develop state-of-the-art **scale-spanning modeling** capabilities: Nanoscale electronic structure & transport up to the macroscale

# Scientific Thrusts for CNMS

CNMS' research is organized under **five related scientific thrusts**, selected to address **grand challenges to understanding and nanotechnology needs**

## Soft and Hybrid Materials [ Michelle Buchanan ]

Organic, hybrid, and interfacial nanophases: Polymers; bio-derived; nanotubes & related; catalysts; fluids; mechanics

## Complex Hard Materials [ Ward Plummer ]

Nano-functional materials: Understanding and using effects of reduced dimensionality, cooperative, and self-organizing behavior

## Nanofabrication [ Mike Simpson ]

**Nanofabrication Research Laboratory --**

Controlled synthesis and directed assembly

Link nanoscale phenomena up to the macroscale

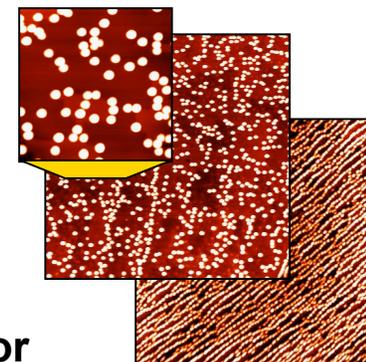
Functionally integrate “soft” and “hard” materials

## Theory, Modeling, Simulation [ Peter Cummings ]

**Nanomaterials Theory Institute --** Grand challenges of “computational nanoscience”: Multi-scale modeling, nanomaterials design, and virtual synthesis

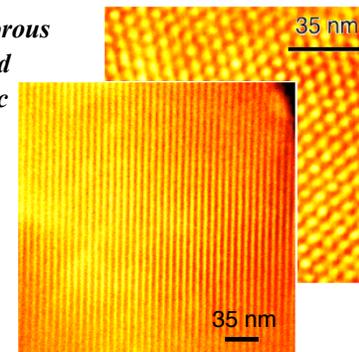
## Nanoscale Imaging and Characterization [ David Joy and Ian Anderson ]

New instruments and methods to **manipulate** nanostructures for properties measurements, with **simultaneous imaging and environmental control**



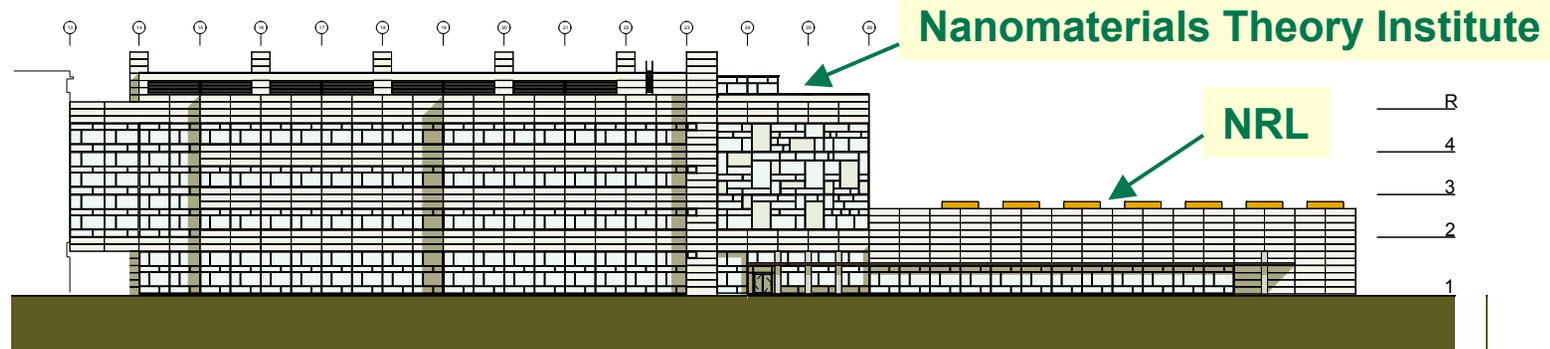
AFM images of Fe nanodots and nanowires on flat and stepped NaCl surfaces (edge length 750 nanometers)

Ordered nanoporous silica synthesized using an organic template



**Enabling Collaborative, Multidisciplinary Research and Nanomaterials Integration**

# Building and Support Facilities



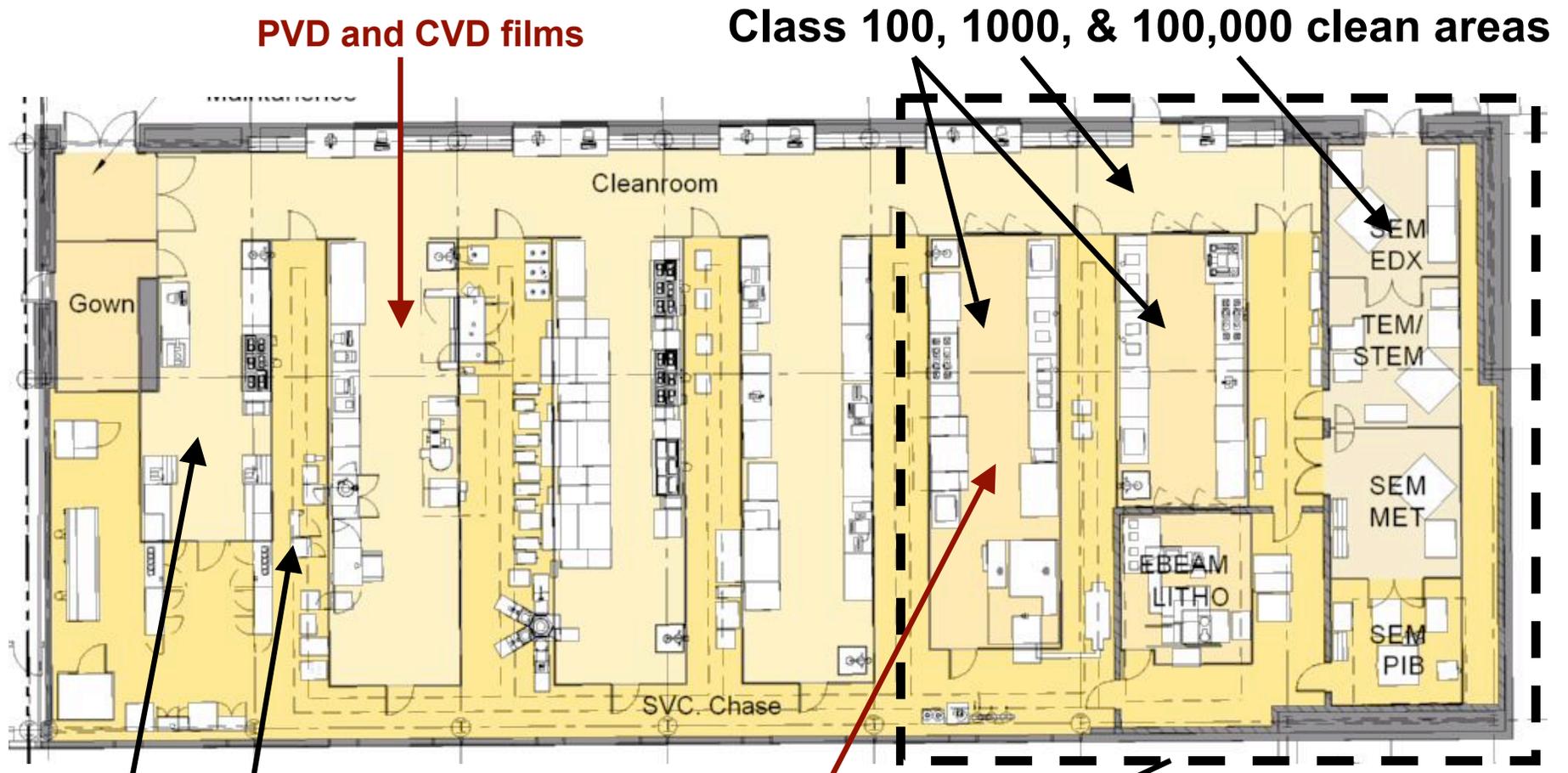
- 80,000 sf: Four levels + Nanofabrication Research Lab (NRL, ~10,000 sf)
- 32 “wet” and “dry” materials synthesis and characterization labs
- Office space for 190 staff and visitors: *Immediately opposite labs to maximize collaborative, multidisciplinary, and educational interactions*
- **NRL:** Clean and environmentally controlled rooms; electron microscopes; nanoscale patterning (e-beam writer / lithography); facilities for manipulation and integration of soft & hard materials
- **CNMS 1<sup>st</sup> floor** (adjacent to NRL): High-resolution scanning probes
- **Nanomaterials Theory Institute:** Offices + lab to access terascale computing facilities of ORNL Center for Computational Sciences (CCS)

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1<sup>st</sup> NSRC User Workshop

# Nanofabrication Research Laboratory



PVD and CVD films

Class 100, 1000, & 100,000 clean areas

Bay/chase configuration

PHOTOLITHOGRAPHY

Electromagnetic, vibration, acoustical (EVA) controlled area



**Cleanroom Bay**

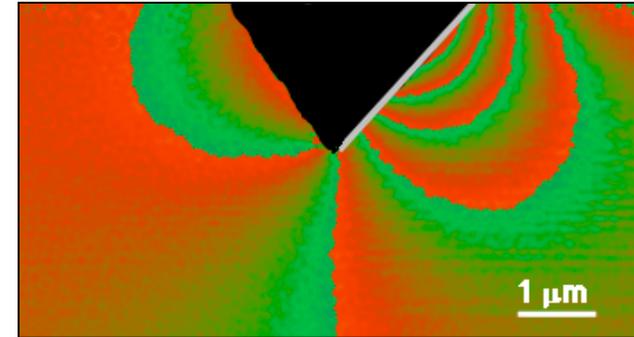


**Tool Move-in Aisle**

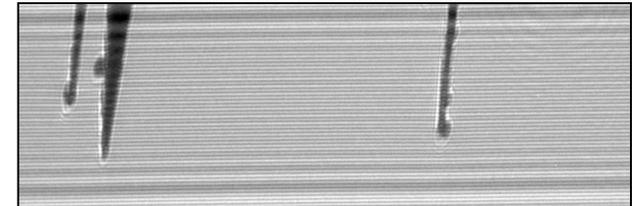
# Nanoscale Imaging & Characterization

## SCIENTIFIC FOCUS AND KEY CAPABILITIES

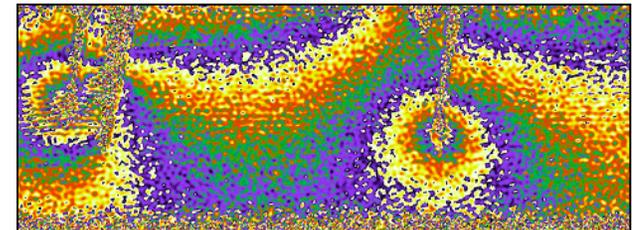
- **Balanced approach for users**
  - **High-resolution, high-throughput instruments**  
Expensive, appropriate for User Center  
“Standard” instruments, can be purchased
  - **Truly novel imaging and measurement tools**  
Near-unique measurement / manipulation  
Attract forefront science and scientists



*Phase image reconstructed from a FETEM hologram shows magnetic fields outside the CoNi layer (shown in gray) on a Magnetic Force Microscope (MFM) tip.*

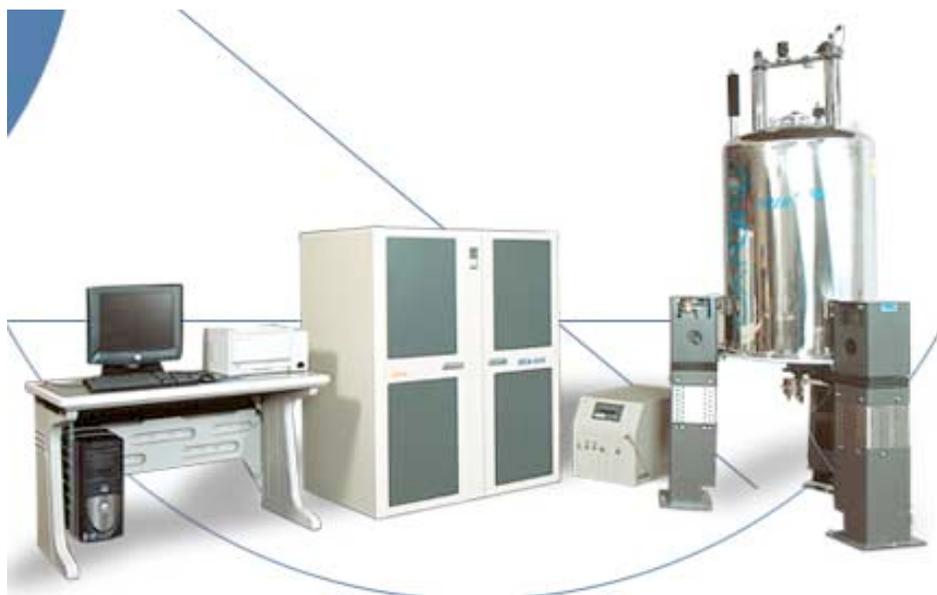


*(ABOVE) Off-axis hologram of carbon nanofibers. (BELOW) The reconstructed pseudo-color phase image shows the equipotentials.*



**Images: Prof. David Joy (ORNL-UT)**

# 600 MHz Nuclear Magnetic Resonance Spectrometer



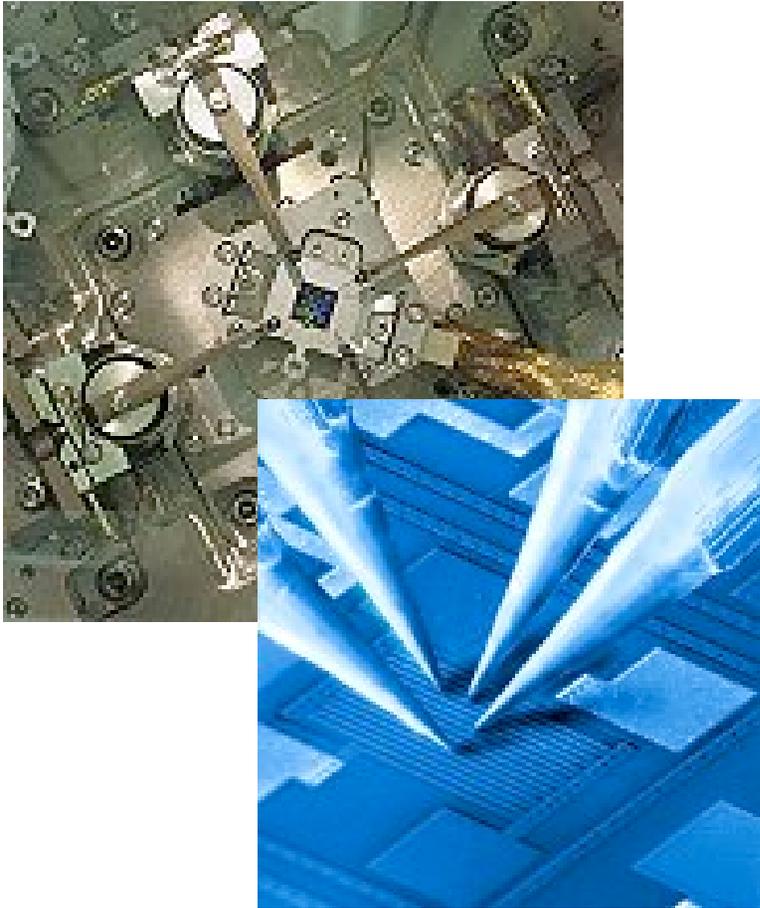
- **Scientific Drivers**

- Critical for **soft materials characterization**
- Best tool for establishing the **connectivity and structure** of organic molecules
- Investigations of the **interface** between block copolymers, organic–inorganic interfaces, biologically-derived materials

- **Capabilities**

- Wide-bore 600 MHz NMR with broadband probes (for  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^2\text{H}$ ,  $^{19}\text{F}$ ,  $^{27}\text{Al}$ ,  $^{29}\text{Si}$ ,  $^{31}\text{P}$ , etc.)
- Analysis of **solid and liquid** samples

# Four-probe Transport Scanning Tunneling Microscope with SEM



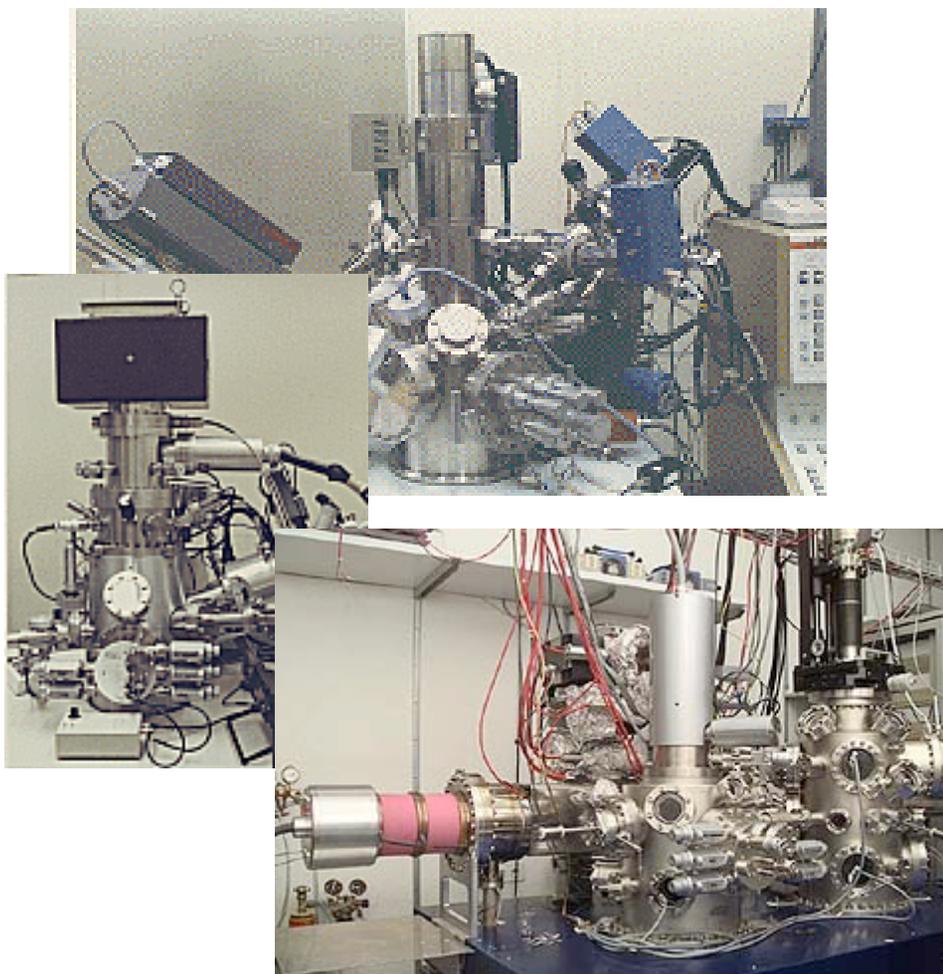
- **Scientific Drivers**

- Temperature-dependent electrical transport measurements of nanoscale objects on surfaces

- **Capabilities**

- SEM resolution  $\sim 5$  nm permits accurate positioning of four tips relative to each other and to nanofeatures of interest
- Four probes operate independently
- Nanofabrication: STM tip-stimulated chemical vapor deposition (CVD)

# High-Resolution Scanning Electron Microscope for (Spin)-Polarized Analysis (SEMPA)

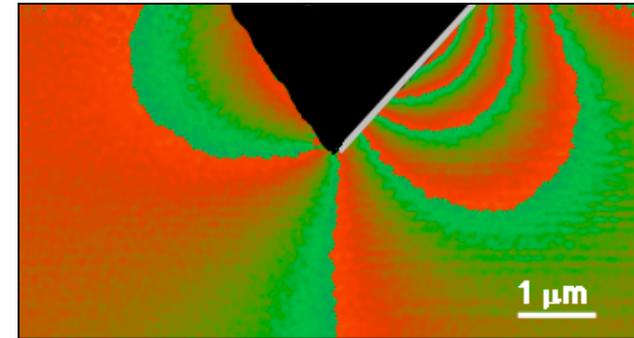


- **Scientific Drivers**
  - Nanometer-scale characterization of magnetic domain structure
- **Capabilities**
  - UHV sample environment and sample preparation system
  - True UHV electron column with 10 - 30 nm resolution
  - Spin detector based on the spin-polarized LEED detector
  - Operates with in-plane magnetic field of 300 mT
  - Elemental analysis of nanostructures via scanning Auger microscopy

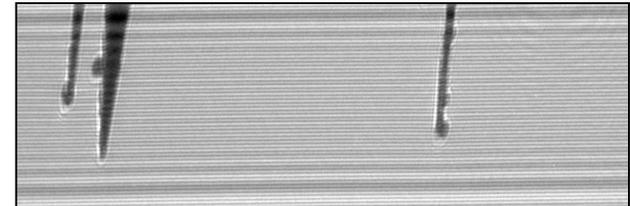
# Nanoscale Imaging & Characterization

## SCIENTIFIC FOCUS AND KEY CAPABILITIES

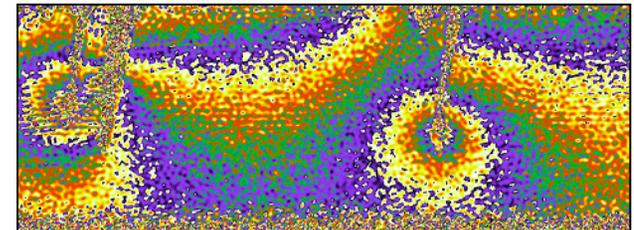
- **Balanced approach for users**
  - High-resolution, high-throughput instruments
  - Truly novel imaging and measurement tools
- **Suite of electron-beam instruments in EVA area of the *Nanofabrication Research Lab***



*Phase image reconstructed from a FETEM hologram shows magnetic fields outside the CoNi layer (shown in gray) on a Magnetic Force Microscope (MFM) tip.*



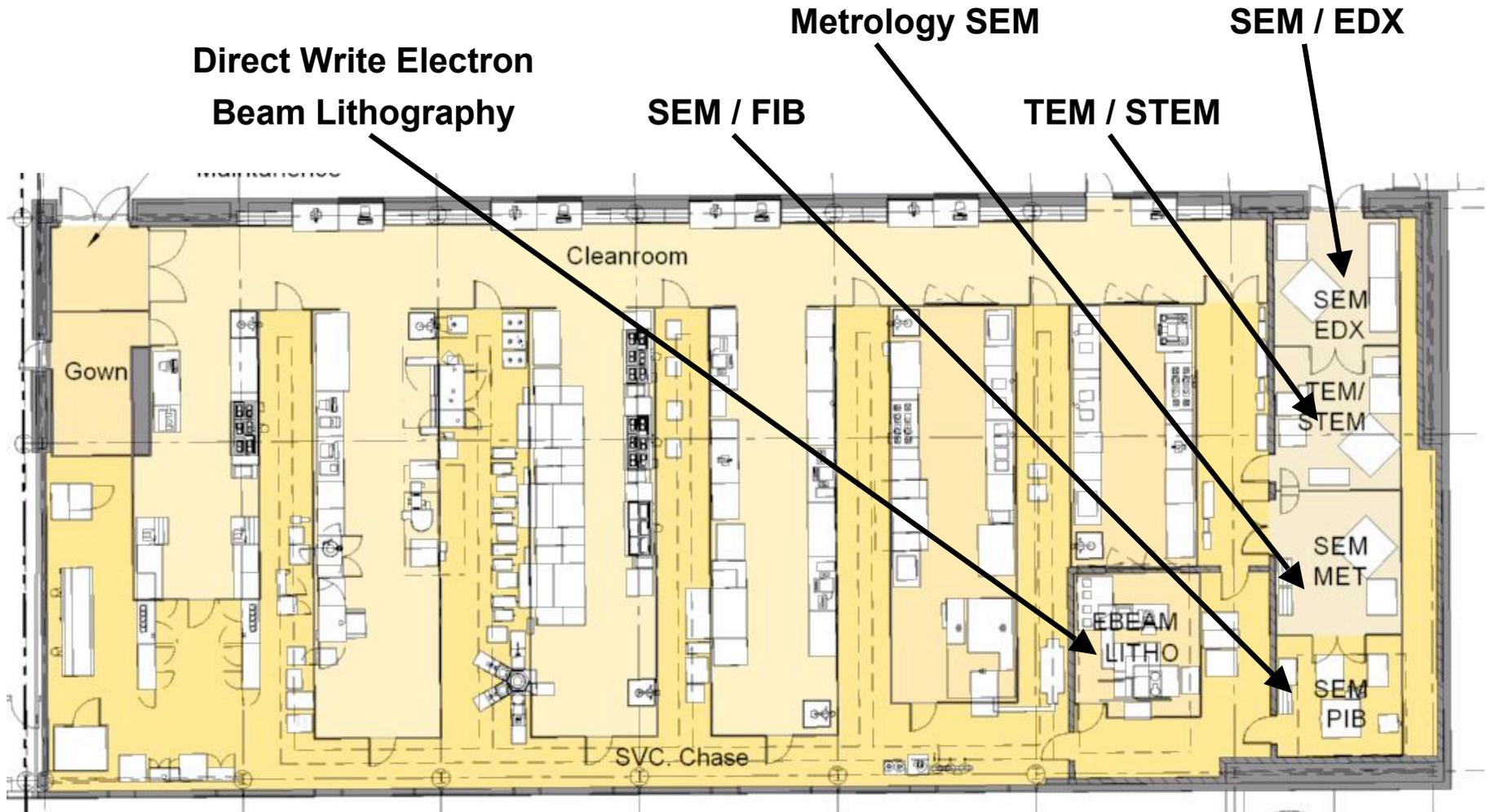
*(ABOVE) Off-axis hologram of carbon nanofibers. (BELOW) The reconstructed pseudo-color phase image shows the equipotentials.*



**Images: Prof. David Joy (ORNL-UT)**

# Nanofabrication Research Laboratory

## Electron Beam Patterning and Materials Characterization

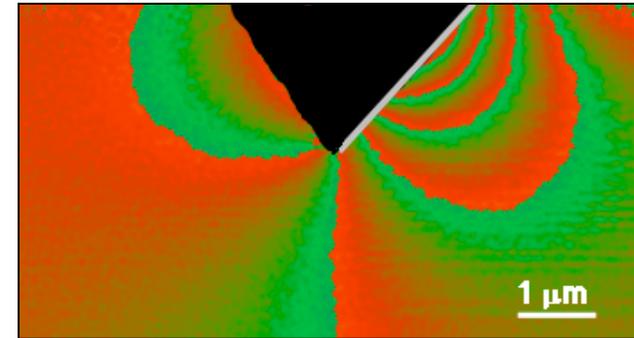


# Nanoscale Imaging & Characterization

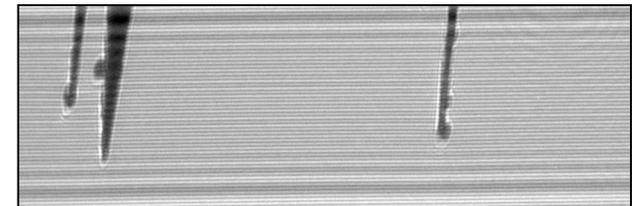
## SCIENTIFIC FOCUS AND KEY CAPABILITIES

- **Balanced approach for users**
    - High-resolution, high-throughput instruments
    - Truly novel imaging and measurement tools
  - **Suite of electron-beam instruments in EVA area of the *Nanofabrication Research Lab***
  - **Combine imaging with *simultaneous* materials manipulation, modification, properties probing**
    - Combine electron microscopy, scanning probes, and focused electron / ion / deposition beams
- [1] HRSEM / scanning probe with **tactile feedback** for *in situ* **mechanical + electrical** properties measurement
  - [2] HR electron holography for quantitative imaging of **nanoscale electric and magnetic fields**
  - [3] Scanning probes in **liquid & gaseous environments**
  - [4] **Environmental SEM and TEM capabilities**

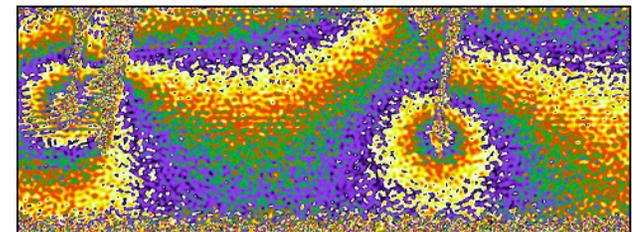
***Electronic, mechanical, chemical, and magnetic properties measurements for nanostructures from hard to very soft***



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***Nanomaterials Theory Institute (NTI)***  
**Stimulate U.S. Leadership in  
Computational Nanoscience**



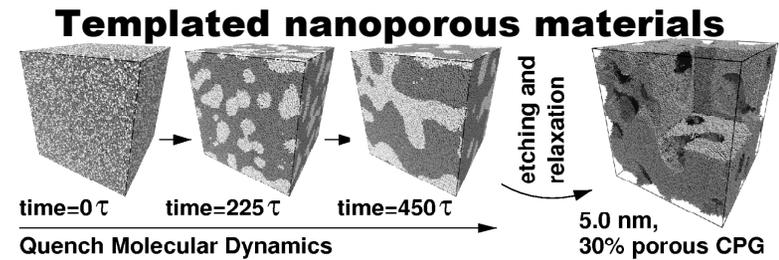
## **VISION AND GOALS**

- **Advance theoretical and computational methodologies** to understand nanoscale materials and phenomena
  - Develop new nanomaterials design and virtual synthesis tools
- Become a premier Center for **dissemination of theory, modeling, and simulation tools** for the nanomaterials sciences

## **APPROACH: *Facilities, Expertise, Intellectual Development***

- Provide access to full range of facilities and staff expertise at ORNL's ***Center for Computational Sciences (CCS)***
- Support users with collaborative expertise through NTI staff, postdocs, visitors + ***Theoretical & Computational Nanoscience Workshops*** program
- Develop state-of-the-art **scale-spanning** modeling capabilities, from nanoscale electronic structure and transport up to the macroscale

# The Nanomaterials Theory Institute (NTI)



## THEORETICAL AND COMPUTATIONAL NANOSCIENCE WORKSHOPS PROGRAM

- **INTELLECTUAL IMPACT:** Provide mechanism for bringing together world leaders to advance computational nanoscience
- “Hands on” tutorials and workshops (typically week-long)
  - **Community-driven content:** Proposals from potential workshop chairs
  - Disseminate new theories, models, methods
  - Instruct junior & senior researchers in their use and foster collaborations

The Model: **CECAM** ([www.cecarn.fr](http://www.cecarn.fr))



- Semester-long special topic(s) research on-site at CNMS / NTI
  - ~ Bring together leaders for longer period of focused collaboration

The Model: **Kavli (NSF) Institute for Theoretical Physics**  
(UCSB, [www.itp.ucsb.edu](http://www.itp.ucsb.edu))



Institute for Theoretical Physics

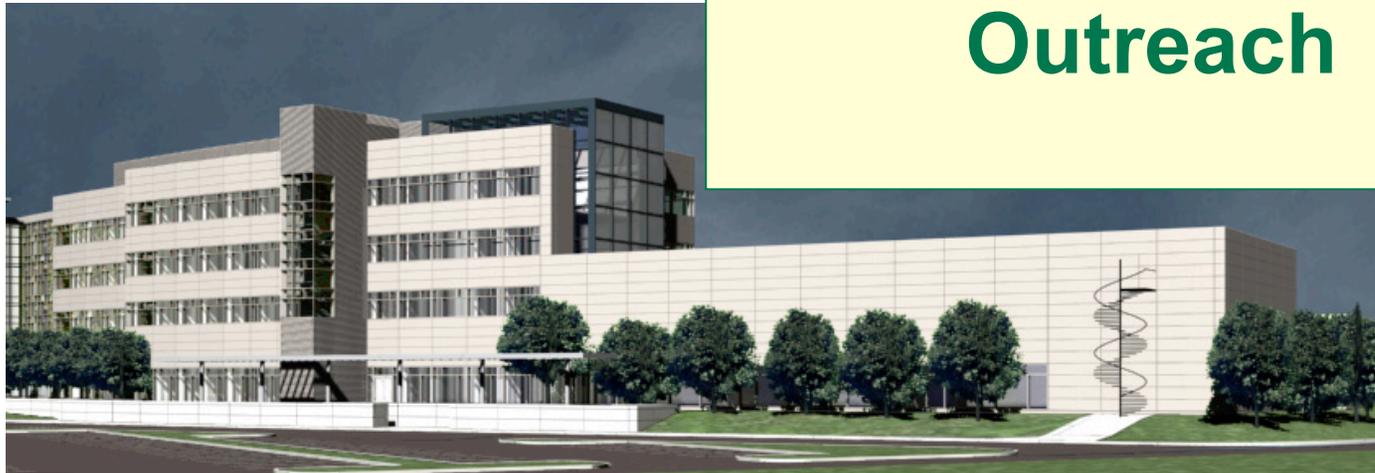
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1<sup>st</sup> NSRC User Workshop



# Plans for CNMS Operational Outreach



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1<sup>st</sup> NSRC User Workshop



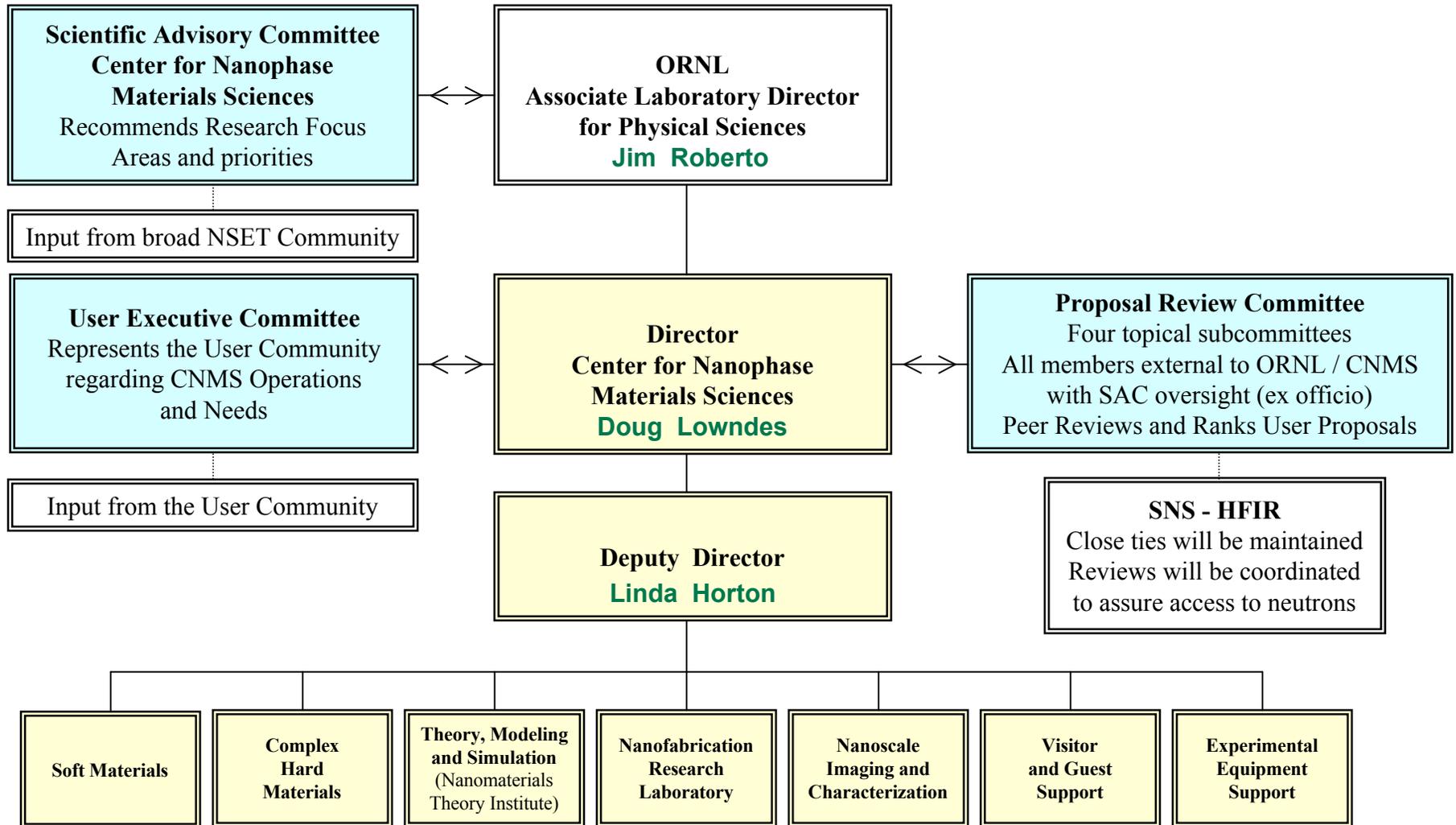
## ***FY2005 Operational Infrastructure***

# **Outreach to Encourage Multidisciplinary Research Education**

## ***CNMS Support for Postdoctoral Scholars***

- **Will hire significant fraction of postdocs with collaborating groups**
  - Partner Access mode, enhancing CNMS capabilities and made available to benefit General Users also
- **Criteria:**
  - Highly motivated research collaborators with own research support
  - Quality and suitability of the Science
  - Scientific Advisory Committee (SAC) recommendations for Research Focus Areas and budget allocations

# Governance of the Center for Nanophase Materials Sciences



Key to Chart colors  
 Yellow: CNMS Leadership Team  
 Blue: External Advisory Committees

# **CNMS' Scientific Advisory Committee (SAC) Appointed**

---

**Professor Jerzy Bernholc**

North Carolina State University

**Professor Daniel E. Morse**

U of California, Santa Barbara

**Professor Jack Crow** (Chair)

Florida State U and National  
High Magnetic Field Lab

**Professor Richard E. Smalley**

Rice University

**Professor Mostafa El-Sayed**

Georgia Institute of Technology

**Professor Julia R. Weertman**

Northwestern University

**Chair, Users' Executive Committee** (ex officio)

ORNL: **Thom Mason (SNS), Malcolm Stocks, Linda Horton**  
(interim)

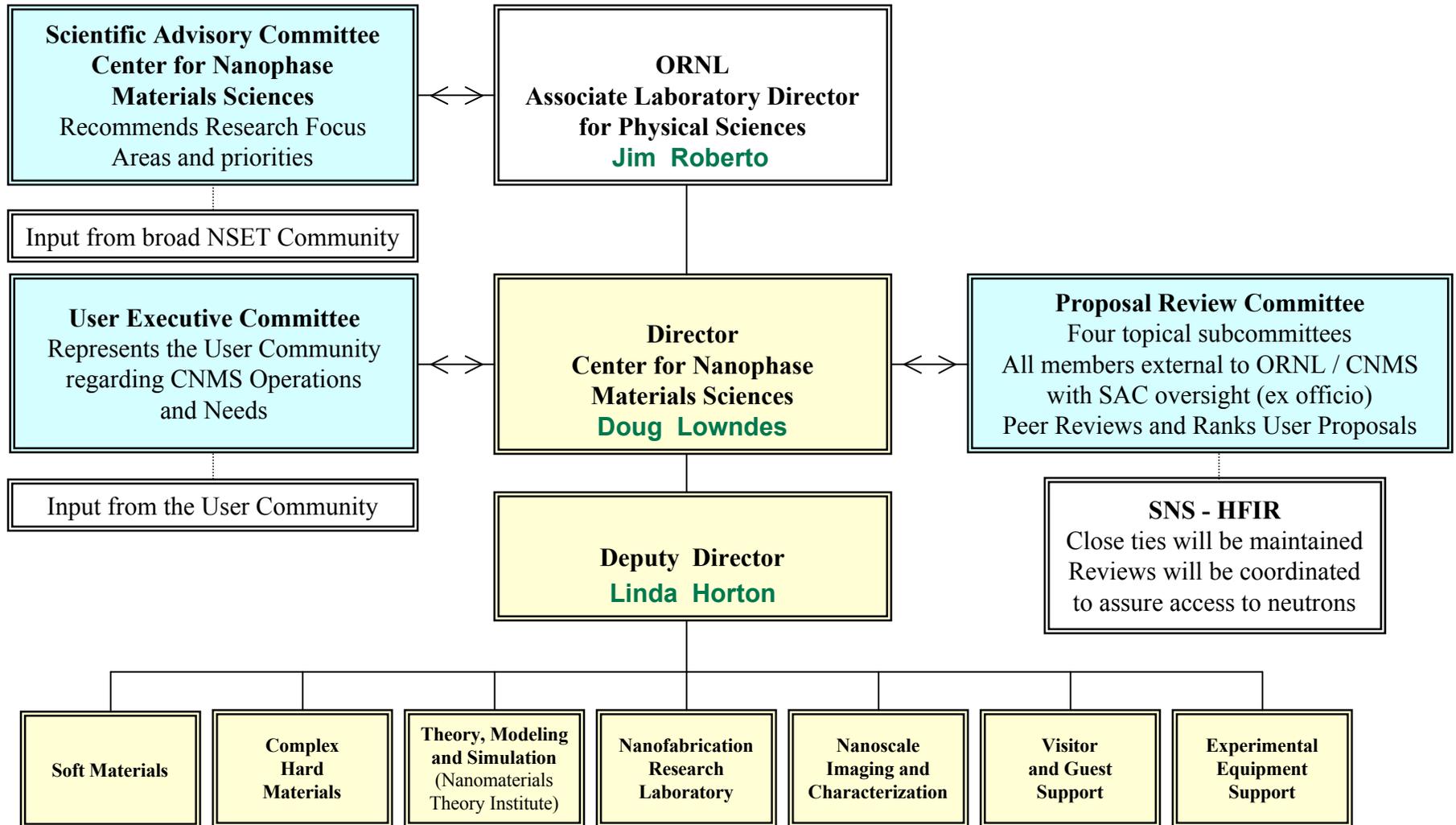
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# *How Will ORNL Initiate a Nanoscience User Program ?*

## *FY2003 “Jump Start” of User Nanoscience Research Activities*



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1<sup>st</sup> NSRC User Workshop



**FY2003 “Jump Start”**

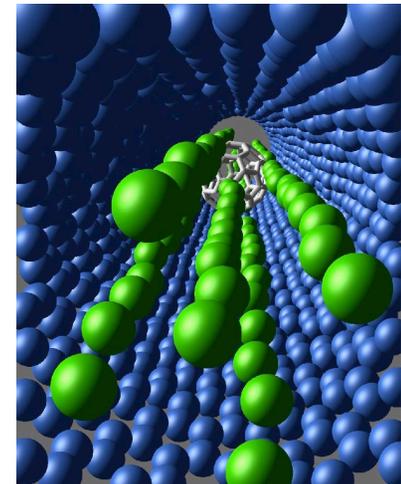
## **ORNL Will Open Several Areas for Nanoscience Research with Users**

### **RATIONALE**

- **CNMS Planning Workshops: Expected strongest user interest**
- **Major strengths** of current ORNL / BES research programs
- **Support for**
  - Controlled synthesis research
  - Broad range of imaging and characterization
  - Theory, modeling, and simulation
  - Nanomaterials design

### **GOAL**

- **Vibrant, interactive, productive user community *before* CNMS opens**



*Computer simulation of a fullerene molecule (white) moving a helium-atom fluid (green) through a carbon nanotube (blue)*

**FY2003 “Jump Start”**

## **Nanoscience Research with Users**

- **Design, Synthesis, and Characterization of Macromolecular Materials**
  - **Materials Focus:** Polymers and biologically-derived or -inspired systems
  - **Grand Challenge:** Design and control macromolecular organization to achieve novel functionalities
- **Controlled Synthesis and Assembly of Functional Nanomaterials**
  - **Materials Focus:** Single- and multi-wall carbon (and eventually other) nanotubes and related composite materials
  - **Grand Challenge:** Understand and control synthesis and functionalization of nanotubes and related structures, to obtain materials with desired physical and chemical properties
- **Initiate Nanomaterials Theory Institute’s targeted Workshops Program**
  - **Two international Theoretical and Computational Nanoscience Workshops**

**FY2003 “Jump Start”**

## **Targeted Workshops Program**

*Nanomaterials Theory Institute’s international*

### **THEORETICAL AND COMPUTATIONAL NANOSCIENCE WORKSHOPS**

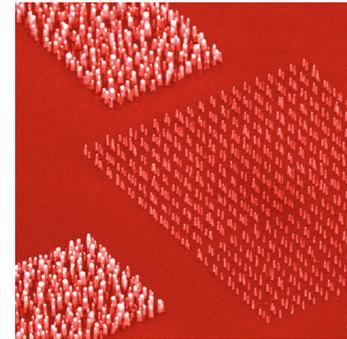
- **“Electronic, Atomistic, and Mesoscale Simulation Methods for Nanoscience”**
  - **Organizers:** Peter Cummings (Vanderbilt) and Sharon Glotzer (Michigan)
  - **Focus:** SIESTA (ab initio MD), LAMMPS (atomistic MD), mesoscale methods
  - **Speakers:** Jose Soler (UAM-Madrid), Emilio Artacho (Cambridge), Julian Gale (Imperial College), Steve Plimpton (SNL), Sharon Glotzer (Michigan)
  - **Date:** Early- to mid-June
- **“Monte Carlo Methods for Classical and Quantum Spin Systems and Beyond: Potential and Limits of the Wang-Landau Algorithm”**
  - **Organizers:** Thomas Schulthess and Malcolm Stocks (ORNL)
  - **Focus:** Wang-Landau density of states algorithm
  - **Speakers:** David Landau (U. Georgia), Matthias Troyer (ETH-Zurich)
  - **Dates:** August 4-8, 2003
- **Workshops will run their example applications “hands on”, using supercomputers of ORNL’s Center for Computational Sciences (CCS)**

**FY2003 “Jump Start”**

# **Outreach to Nanoscience User Community**

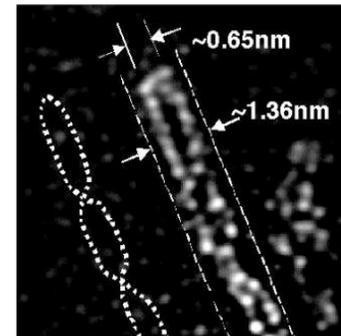
- **Nanofabrication:** Interim nanofabrication lab for users

- Training / supervision for new users
- Skilled technicians for some tasks and/or users
- Communication and enforcement of safe-use and clean-use policies



- **Nanoscale Imaging and Characterization**

- Nanoscience user access to high-resolution electron microscopy, analysis, and scanning-probe instruments in SHaRE & HTML user programs



*Electron microscopy reveals a double helix chain of iodine atoms inside a carbon nanotube*



# Center for Nanophase Materials Sciences

## PROJECT SITE

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Monday, February 10, 2003

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- [Procurement](#)
- [Project Controls](#)
- [Quality Control](#)





[www.cnms.ornl.gov](http://www.cnms.ornl.gov)