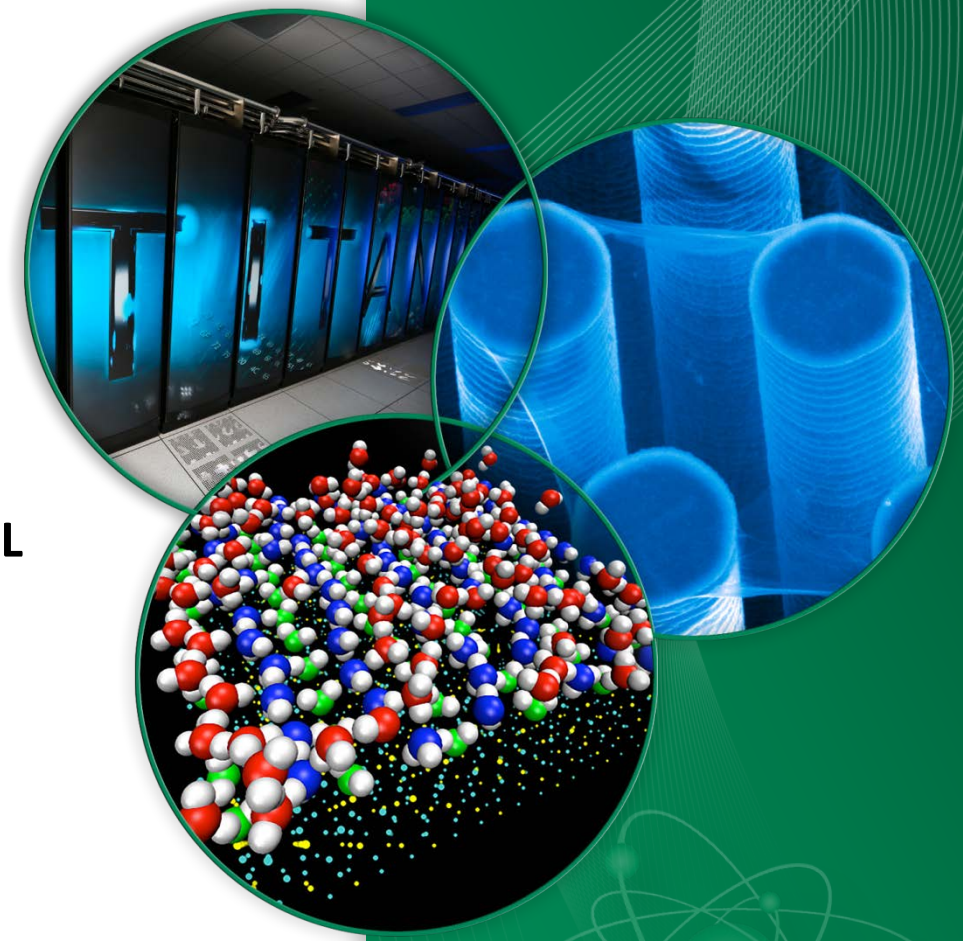
Center for Nanophase Materials Sciences:

a Strategic Overview



Presented via video link to

BIOSYSTEMS, ENERGY, AND CULTURAL HERITAGE:
MATERIALS ENHANCEMENT FOR TECHNOLOGICAL APPLICATION

Università di Roma Tor Vergata
July3rd, 2013

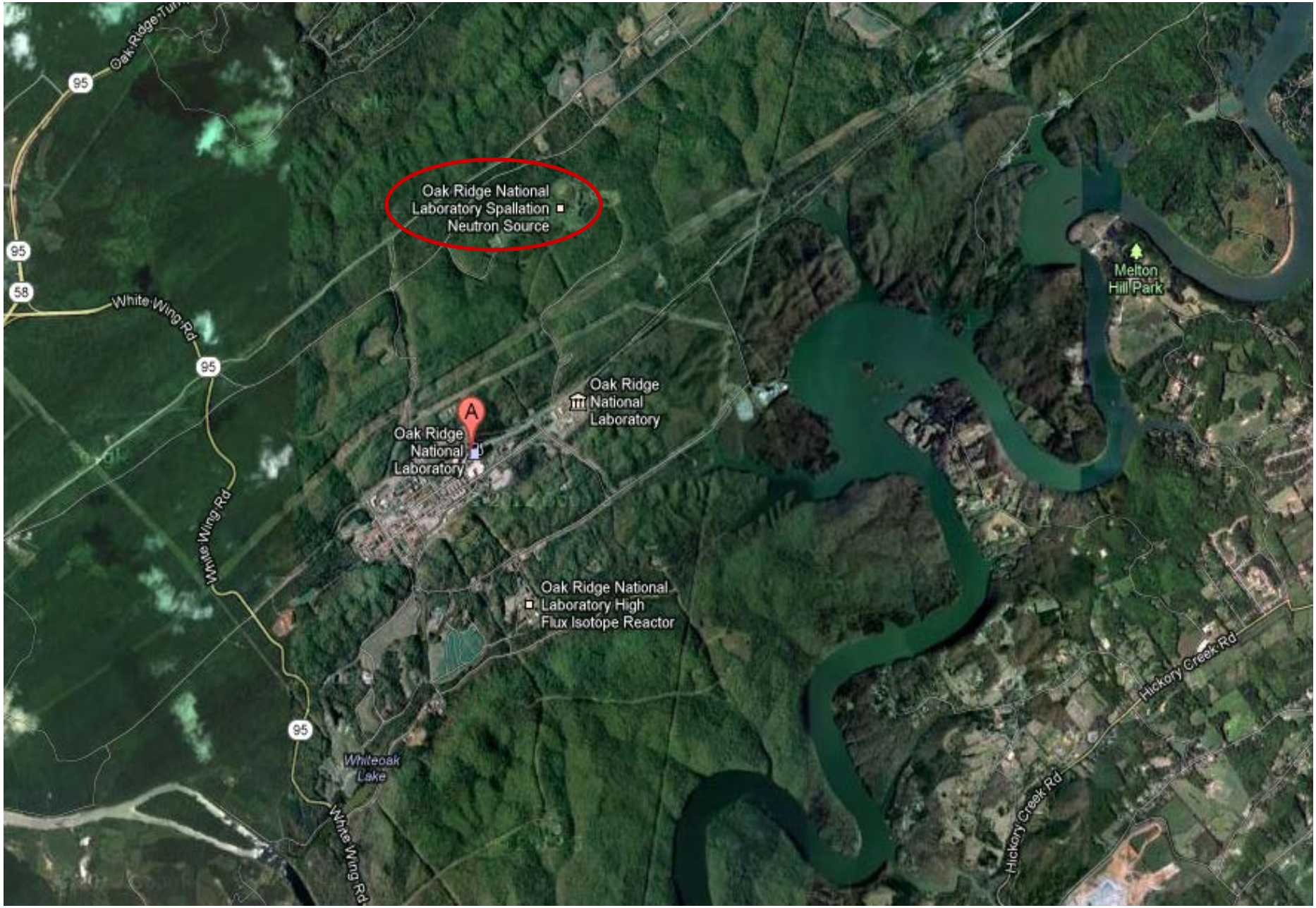
Today, ORNL is DOE's largest science and energy laboratory

- $1.4B budget
- 4,350 employees
- 3,900 research guests annually
- $350 million invested in modernization
- Worlds most powerful open scientific computing facility
- Nation's largest concentration of open source materials research
- Nation's most diverse energy portfolio
- Operating the world's most intense pulsed neutron source
- Managing the billion-dollar U.S. ITER project

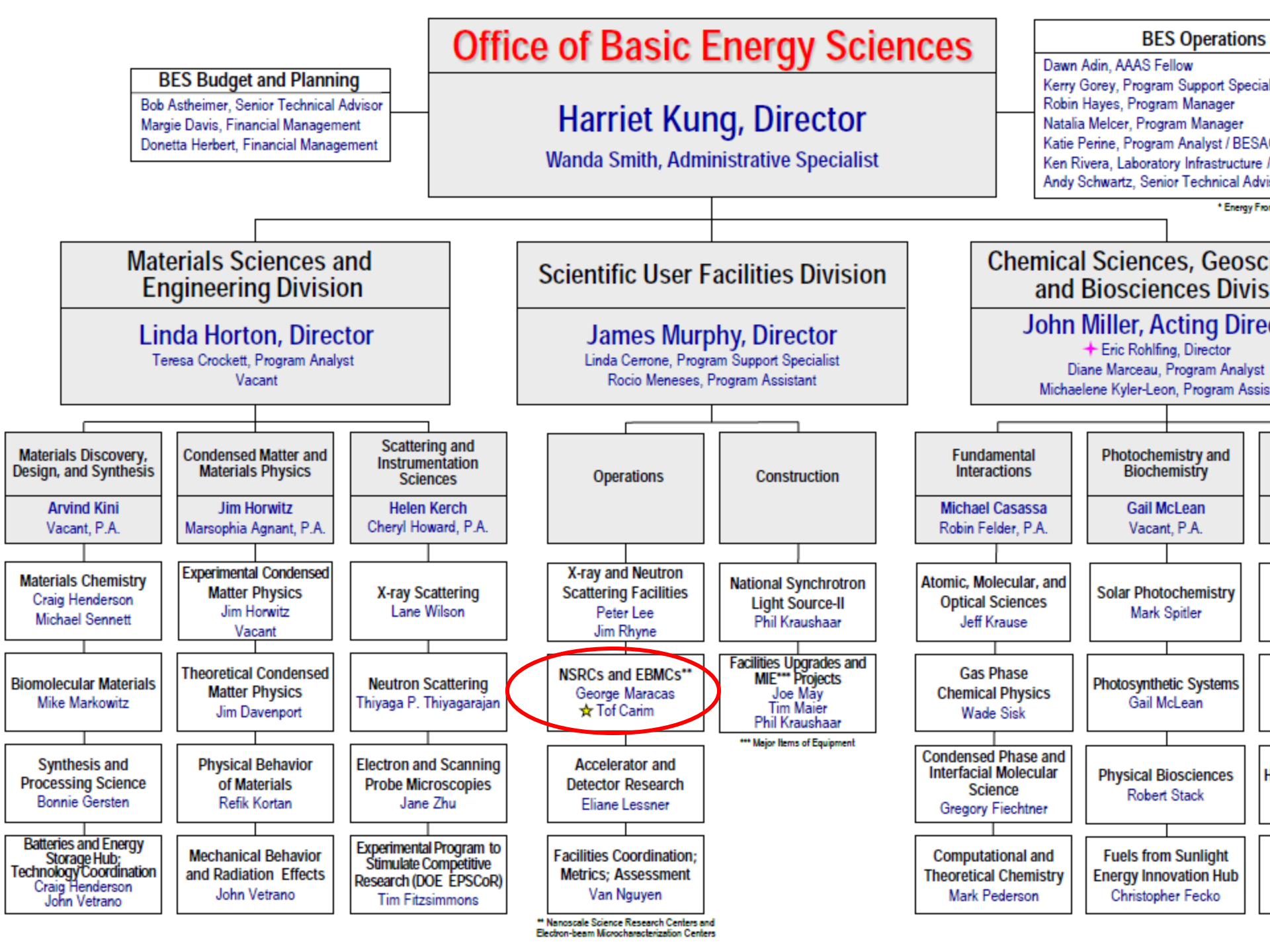
Center for Nanophase Materials Sciences
AT OAK RIDGE NATIONAL LABORATORY

OAK RIDGE National Laboratory

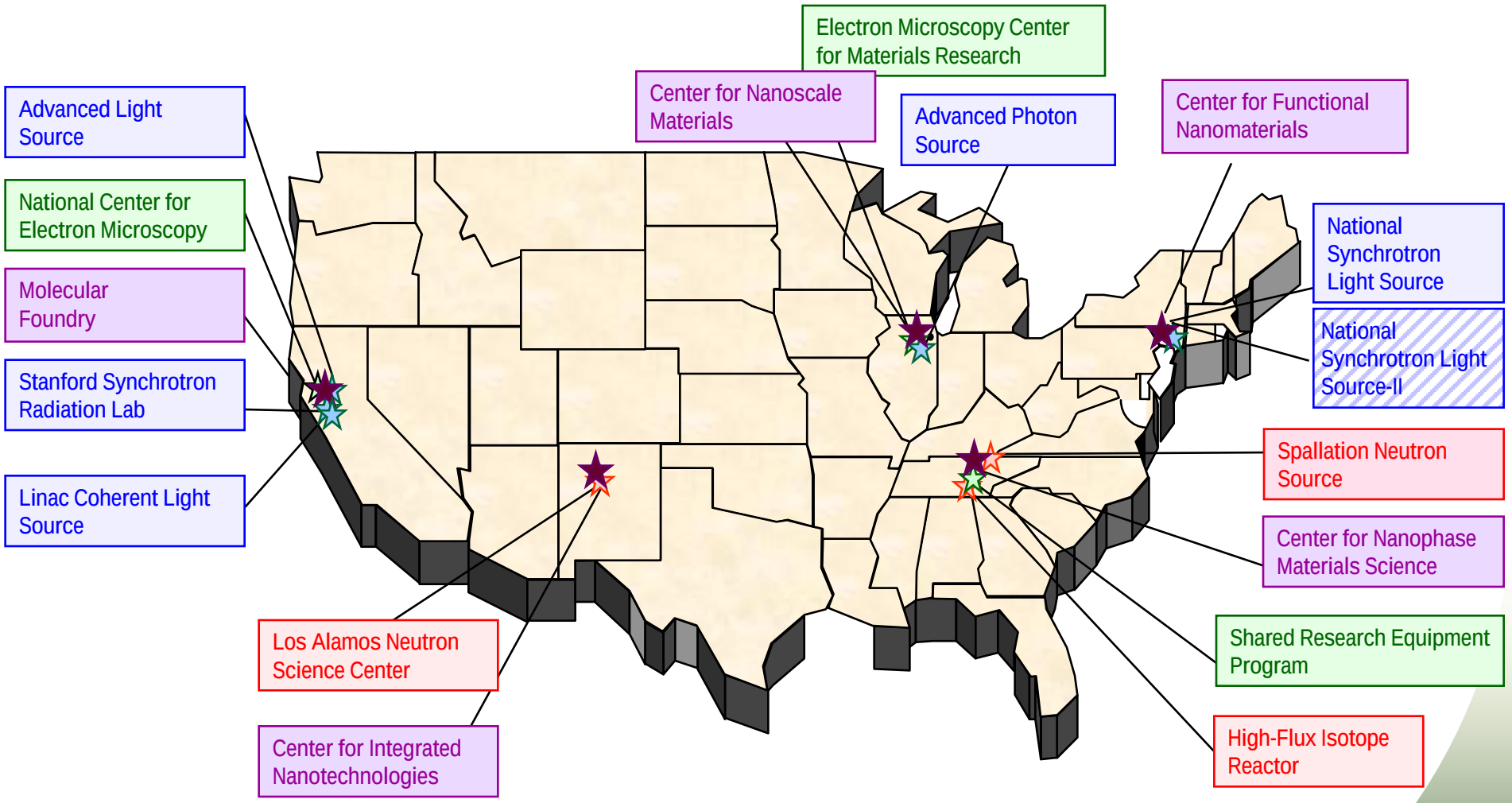
CNMS at ORNL


Oak Ridge National Laboratory Spallation Neutron Source
Oak Ridge National Laboratory
Oak Ridge National Laboratory
Oak Ridge National Laboratory High Flux Isotope Reactor
Melton Hill Park
White Wing Rd
Hickory Creek Rd
Whiteoak Lake
95
58

CNMS – Aerial View


Office of Basic Energy Sciences
Harriet Kung, Director
Wanda Smith, Administrative Specialist
BES Budget and Planning
Bob Astheimer, Senior Technical Advisor
Margie Davis, Financial Management
Donetta Herbert, Financial Management
BES Operations
Dawn Adin, AAAS Fellow
Kerry Gorey, Program Support Special
Robin Hayes, Program Manager
Natalia Melcer, Program Manager
Katie Perine, Program Analyst / BESA
Ken Rivera, Laboratory Infrastructure
Andy Schwartz, Senior Technical Advi
* Energy Fro
Materials Sciences and Engineering Division
Linda Horton, Director
Teresa Crockett, Program Analyst
Vacant
Scientific User Facilities Division
James Murphy, Director
Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant
Chemical Sciences, Geosc and Biosciences Divis
John Miller, Acting Dire
Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-Leon, Program Assis
Materials Discovery, Design, and Synthesis
Arvind Kini
Vacant, P.A.
Condensed Matter and Materials Physics
Jim Horwitz
Marsophia Agnant, P.A.
Scattering and Instrumentation Sciences
Helen Kerch
Cheryl Howard, P.A.
Operations
Construction
Fundamental Interactions
Michael Casassa
Robin Felder, P.A.
Photochemistry and Biochemistry
Gail McLean
Vacant, P.A.
Materials Chemistry
Craig Henderson
Michael Sennett
Experimental Condensed Matter Physics
Jim Horwitz
Vacant
X-ray Scattering
Lane Wilson
X-ray and Neutron Scattering Facilities
Peter Lee
Jim Rhyne
National Synchrotron Light Source-II
Phil Kraushaar
Atomic, Molecular, and Optical Sciences
Jeff Krause
Solar Photochemistry
Mark Spitler
Biomolecular Materials
Mike Markowitz
Theoretical Condensed Matter Physics
Jim Davenport
Neutron Scattering
Thiyaga P. Thiyagarajan
NSRCs and EBMCs**
George Maracas
Tof Carim
Facilities Upgrades and MIE*** Projects
Joe May
Tim Maier
Phil Kraushaar
*** Major Items of Equipment
Gas Phase Chemical Physics
Wade Sisk
Photosynthetic Systems
Gail McLean
Synthesis and Processing Science
Bonnie Gersten
Physical Behavior of Materials
Refik Kortan
Electron and Scanning Probe Microscopies
Jane Zhu
Accelerator and Detector Research
Eliane Lessner
Condensed Phase and Interfacial Molecular Science
Gregory Fiechtner
Physical Biosciences
Robert Stack
Batteries and Energy Storage Hub; Technology Coordination
Craig Henderson
John Vetrano
Mechanical Behavior and Radiation Effects
John Vetrano
Experimental Program to Stimulate Competitive Research (DOE EPSCoR)
Tim Fitzsimmons
Facilities Coordination; Metrics; Assessment
Van Nguyen
Computational and Theoretical Chemistry
Mark Pederson
Fuels from Sunlight Energy Innovation Hub
Christopher Fecko
** Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers

BES Scientific User Facilities: Resources for Energy Research



Nanoscale Science Research Centers

Center for Functional Nanomaterials (Brookhaven National Laboratory)

Center for Nanoscale Materials (Argonne National Laboratory)

Molecular Foundry (Lawrence Berkeley National Laboratory)

Center for Nanophase Materials Sciences (Oak Ridge National Laboratory)

Center for Integrated Nanotechnologies (Sandia & Los Alamos National Labs)

Research Capabilities/ Groups

CENTER FOR NANOPHASE MATERIALS SCIENCES

Sean Smith,* Director
Amanda Zetans, Division Administrative Support
Tony Haynes, User Program Manager
Viviane Schwartz,* User Program Staff
*Sandy Lowe,** User Program Administrative Assistant

Adam Rondinone,* Industry Liaison
Kunlun Hong,* Neutron Science Liaison

Theme Leads
Sergei Kalinin*
Electronic and Ionic Functionality on the Nanoscale
Bobby Sumpter*
Functional Polymer and Hybrid Architectures
Mike Simpson*(1)
Collective Phenomena in Nanophases

Operations/Support
Kara Clayton, Finance
Scott Hollenbeck, Operations Manager(6)
*Lisa Goins**
Jason Taylor(4)
Michele Lusk, HR Manager

*Multiple Capacity
(1) Joint Faculty
(2) Technician
(3) Subcontractor
(4) Lab Waste Services
(5) UT postdoc
(6) Integrated Res. Ops
(7) Wigner Fellow
(8) Clean Room Task Lead
(9) Polymers Task Lead
(10) Catalysis Task Lead
(11) Optoelectronic Task Lead

Imaging and Nanoscale Characterization

Art Baddorf*
*Lisa Goins**

Nina Balke
Zheng Gai
Ilia Ivanov*
Stephen Jesse
Sergei Kalinin*
An-Ping Li
Peter Maksymovych
Minghu Pan
Alexander Tselev(3)

Postdocs: Tom Arruda, Alex Belianinov, Jennifer Black, Corentin Durand, Simon Kelly, Wenzhi Lin, Mahmut Okatan, Jewook Park, Geoffrey Rojas, Evgheni Strelcov, Rama Vasudevan

Nanomaterials Synthesis and Functional Assembly

Dave Geohegan
*Carole Holbrook**
*Erica Lohman**

Mike Biegalski
Pam Fleming(2)
Ilia Ivanov*
Igor Merkulov(3)
Alex Puretzky
Chris Rouleau
Kai Xiao

Deanna Pickel
Peter Bonnesen
Kunlun Hong*
Mike Kilbey(1)
Chengdu Liang*
Brad Lokitz
Jamie Messman
David Uhrig(4)

Adam Rondinone*(10)
Jihua Chen
Sheng Dai*
David Joy(1)
Jong Keum
Chengdu Liang*
Steve Overbury
Michelle Pawel(4)
Viviane Schwartz
Zili Wu

Postdocs: Suk-Kyun Ahn, Balaka Barkakaty, Lu Cai, Yan Chen, Phani Dathar, Eric Formo, Brad Habenicht, Youjun He, Xufan Li, Ming-Wei Lin, Masoud Mahjouri-Samani, Liang Qiao, Nathan Ramanathan, Ezhiyl Rangasamy, Gayatri Sahu, Ming Shao, Leah Sheridan, Jiahua Zhu,

Nanofabrication

Mike Simpson*(1)
Jessica Garner

Pat Collier
Mitch Doktycz
Jason Fowlkes
Ivan Kravchenko
Dayrl Briggs(2)(8)
Dale Hensley(4)
Kevin Lester(2)
Bernadeta Srijanto(3)

Nick Lavrik
Philip Rack(1)
Scott Retterer
Elizabeth Vargis(5)

Postdocs: Rebecca Agapov, Jonathan Boreyko, Ryan Hansen

Students: Charles Chin, Paul Mruetusatorn, Liz Norred

Nanomaterials Theory Institute

Bobby Sumpter*
*Erica Lohman**

Ariana Beste(3)
Gonzalo Alvarez-Campot
Miguel Fuentes-Cabrera
Brandon Cook(3)
Peter Cummings(1)
Panchapakesan Ganesh

Monojoy Goswami(3)
Jingsong Huang
Jacek Jakowski(3)
Paul Kent
Rajeev Kumar
Thomas Maier

Matt Reuter(7)
Sean Smith*
Michael Summers
Mina Yoon
Xiaoguang Zhang

Postdocs: Georgios Barmparis, Khaled Al-Hassanieh, Phani Dathar*, Changwon Park, Julian Rincon, Yu Xie, Jia Zhou

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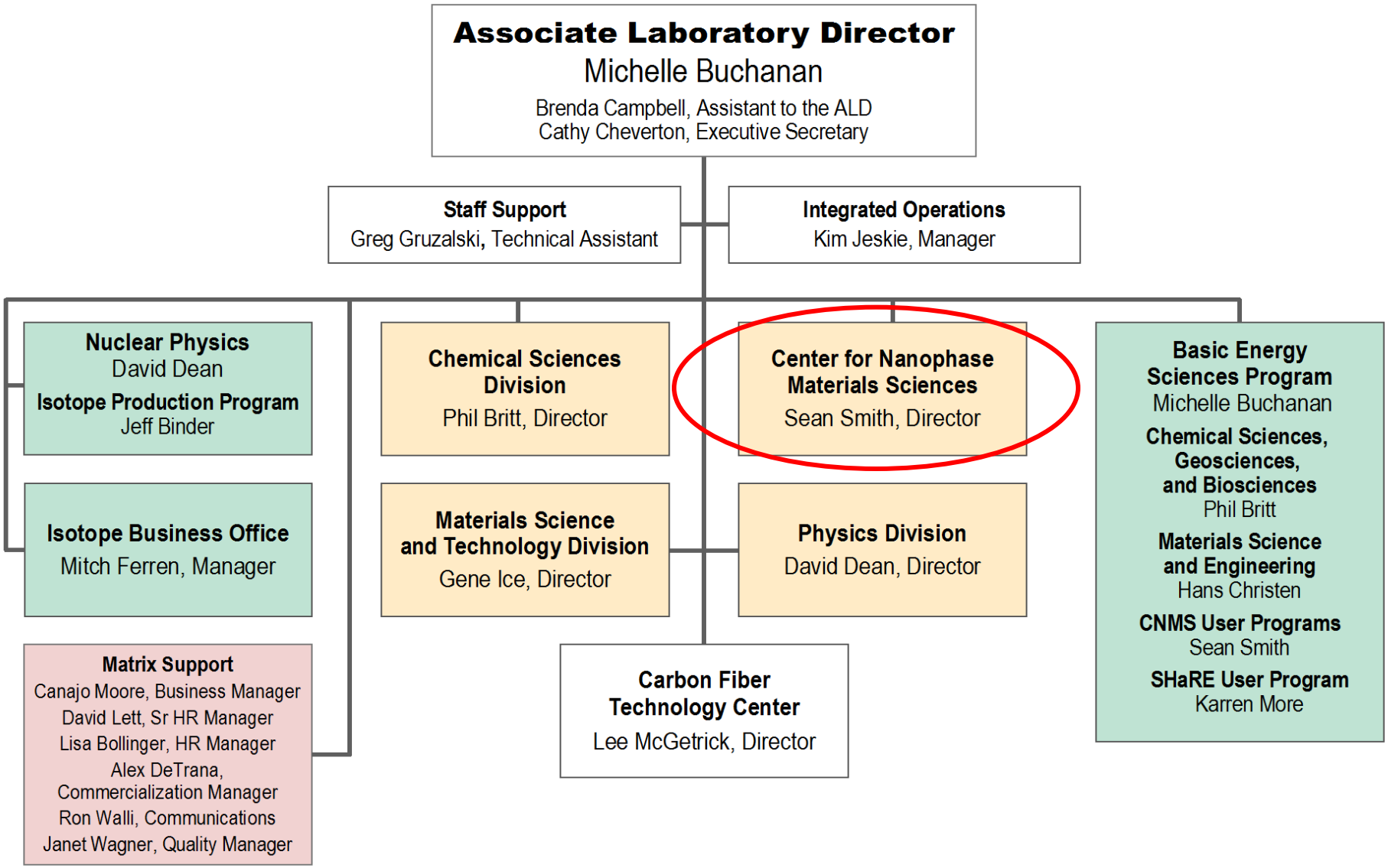
Where are we at ORNL?

Physical Sciences Directorate

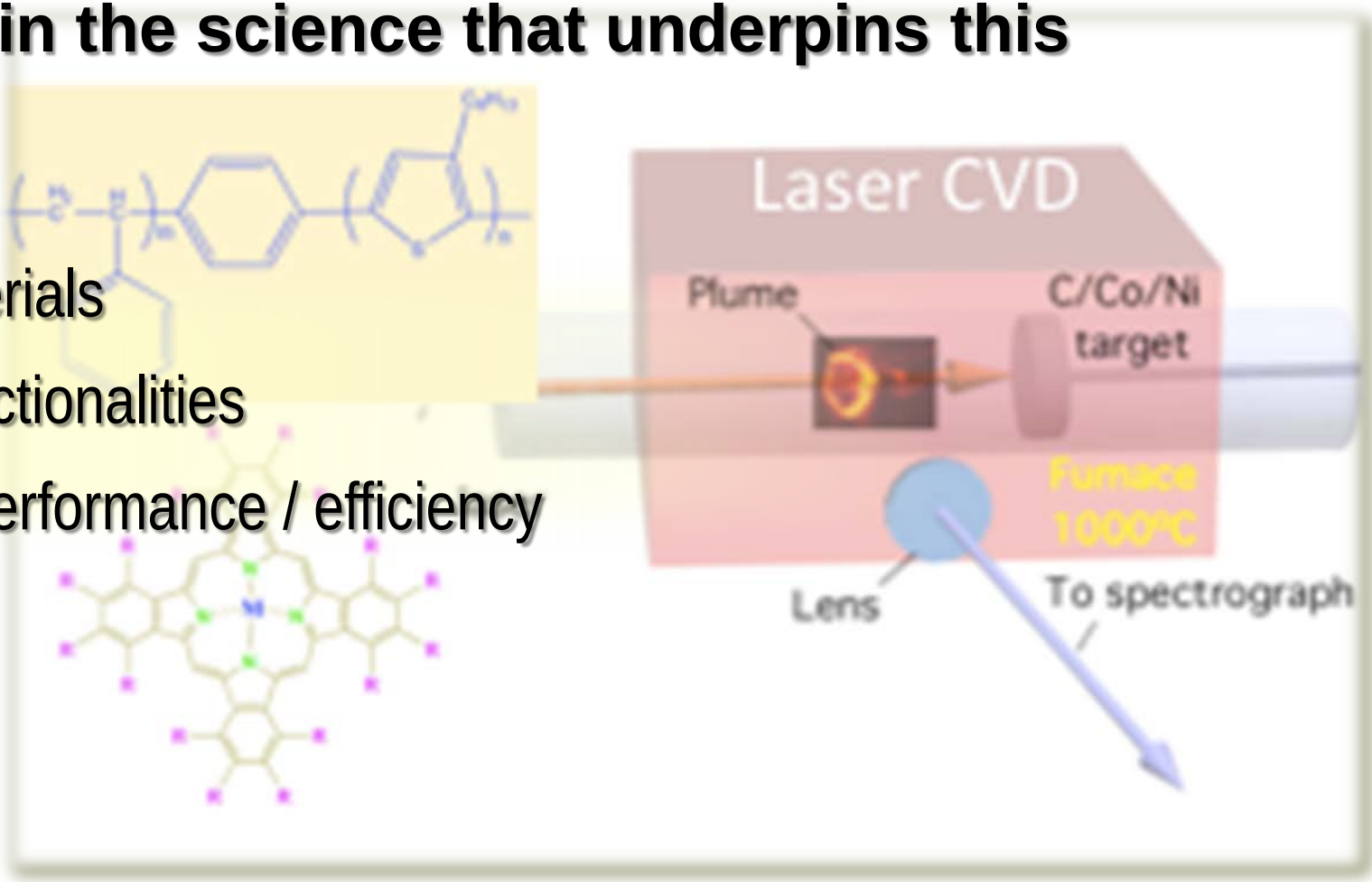


Disruptive Materials

Are the materials that will support or enable disruptive technologies.

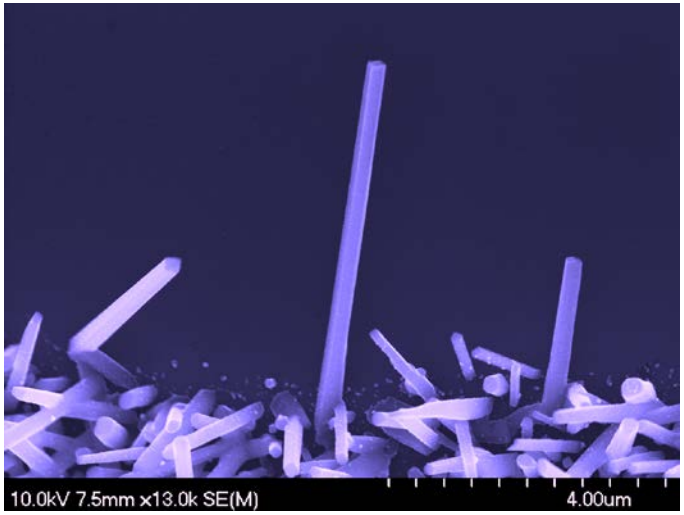
The Physical Science Directorate is heavily engaged in the science that underpins this quest:

- New materials
- Novel functionalities
- Greater performance / efficiency

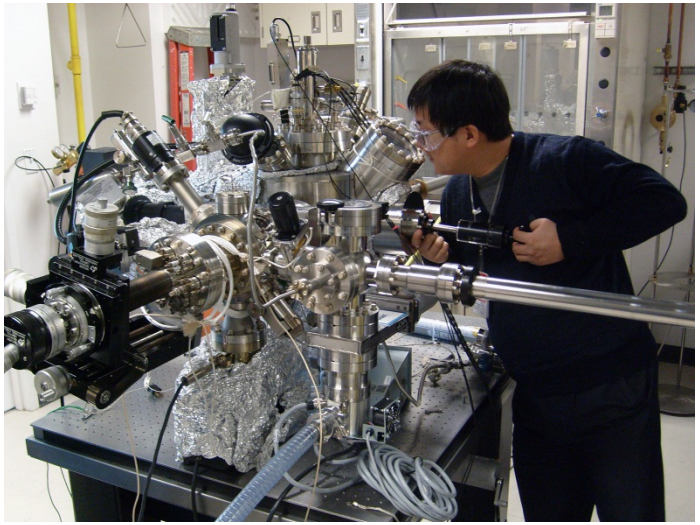


The Quest for New Materials

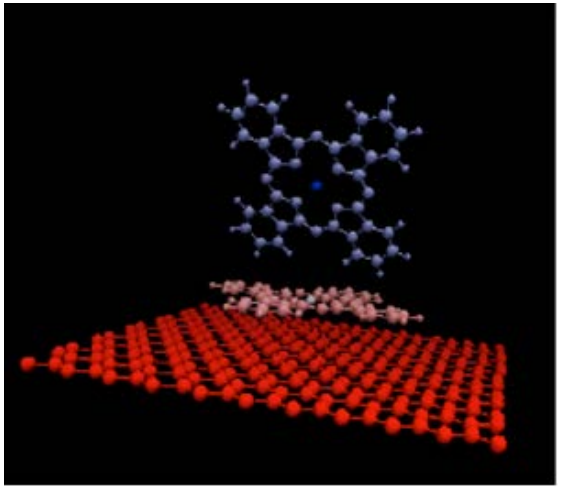
Synthesis



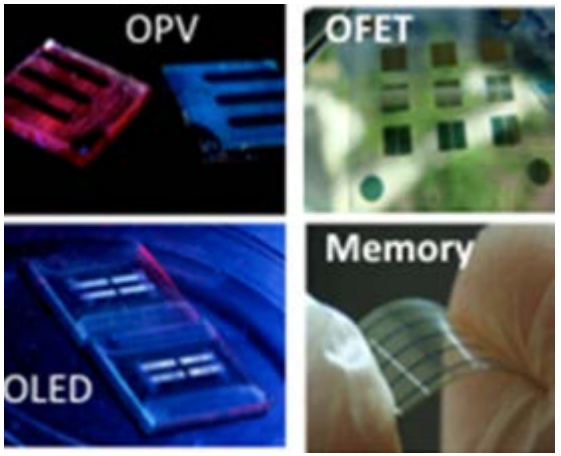
Characterization



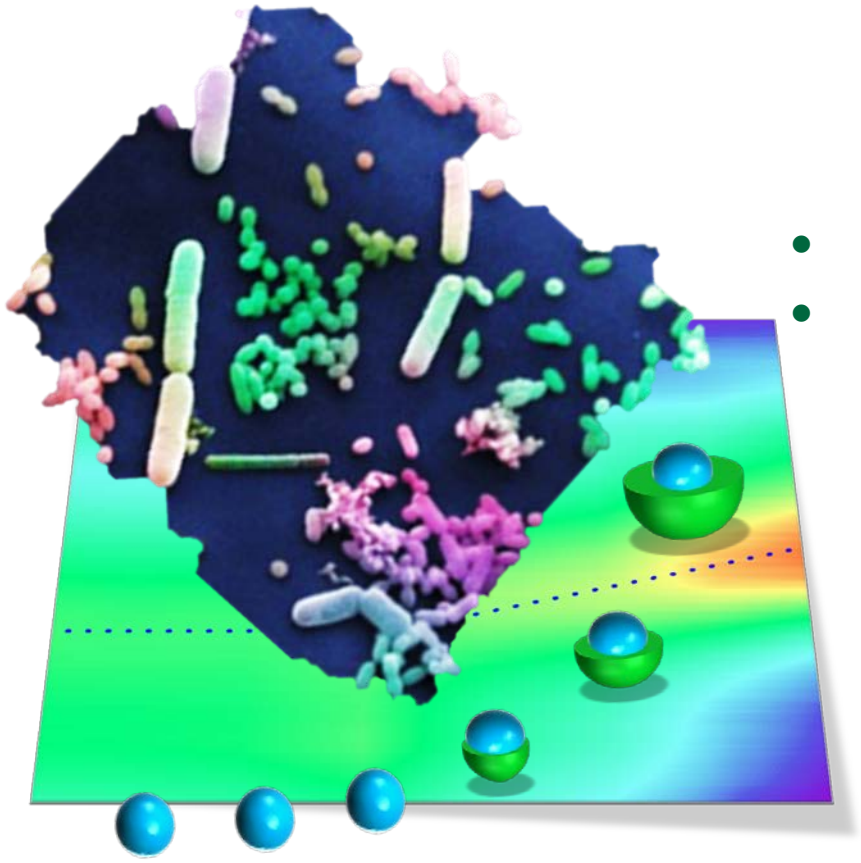
Theory / Simulation



Testing Functionality



Can we use nanotechnology to mimic biosynthesis of nanoparticles?



Formation of core-shell like structure of CdS nanoparticles by nanofermentaiton
J. Won (submitted)

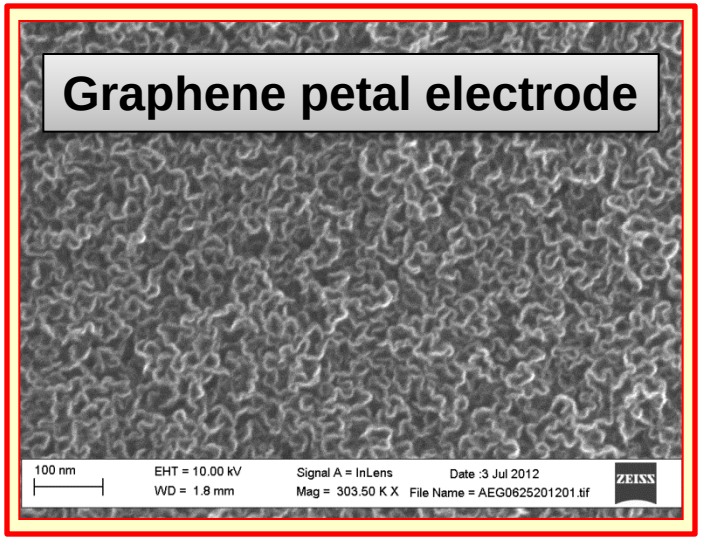
- **A Broad variety of nanoparticles relevant to Solid State Lighting Photovoltaic and Energy storage have been made at ORNL.**
  - **Binary**
  - **Ternary**
  - **Complex(core-shell)**
- ***Low temperature, low cost, scalability***
- **Unsolved mystery- the mechanism of reduction?**
  - **How multi-electron reduction is achieved by bacteria?**
  - **What is the role of cell membrane morphology?**
  - **We have an evidence that in the presence of dead bacteria reduction still takes place!**
  - **What organics are left on the surface of the nanoparticles?**

Scientific question: What can we learn from the nanofermentation and how we can mimic it using nanostructured electrodes/membranes?

Can a nanoscale-patterned electrode offer additional control of electronic and ionic functionalities?

Research approach:

- Surface patterning through deposition of pre-formed nanostructure or seeded growth
- Traditional nanofabrication or etching
- Block – copolymer assembly



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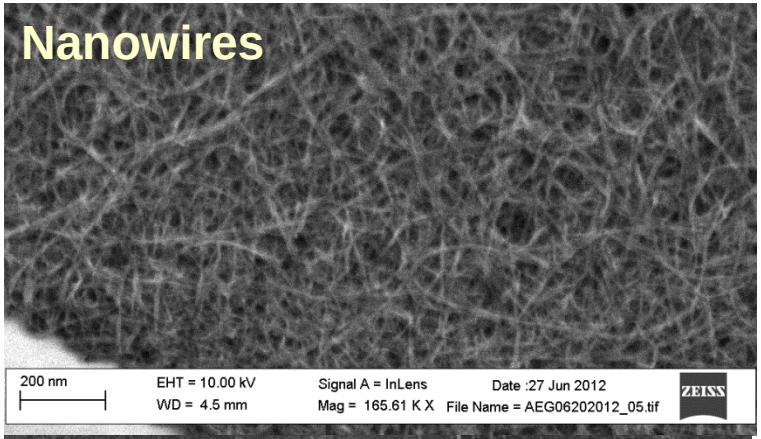
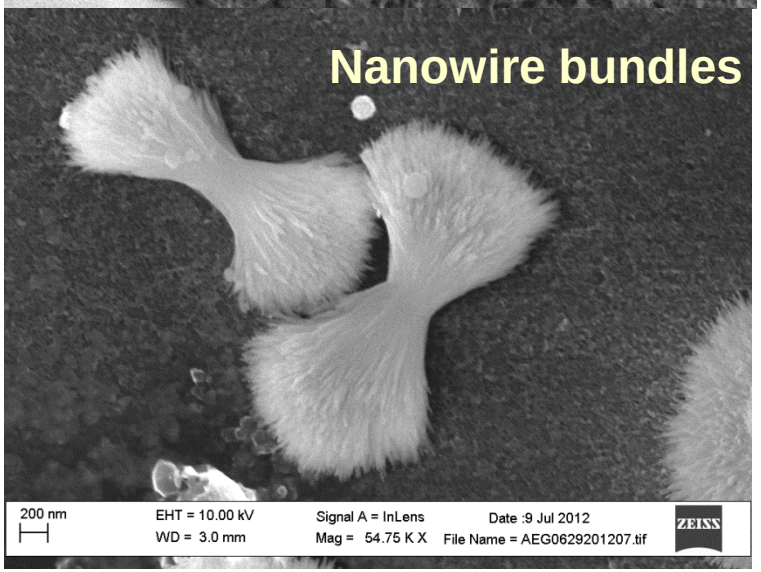
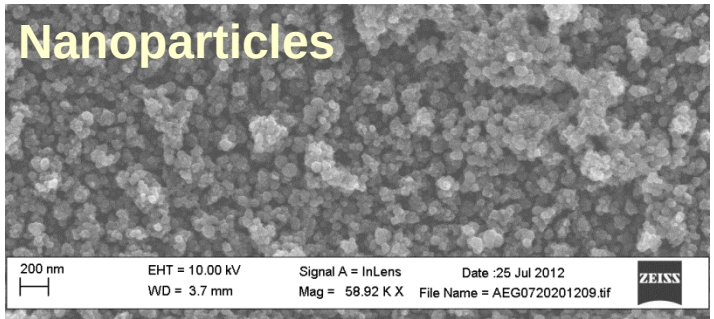
A remarkable variety of CdS nanostructures can be made!

- Electrode promotes local reactions on graphene edges.
- Same electrode and reagents for all structures below.
- Varied surfactant and template chemistry
- Better control – and no need to sustain live bacteria!
- Now looking at more complex inorganics







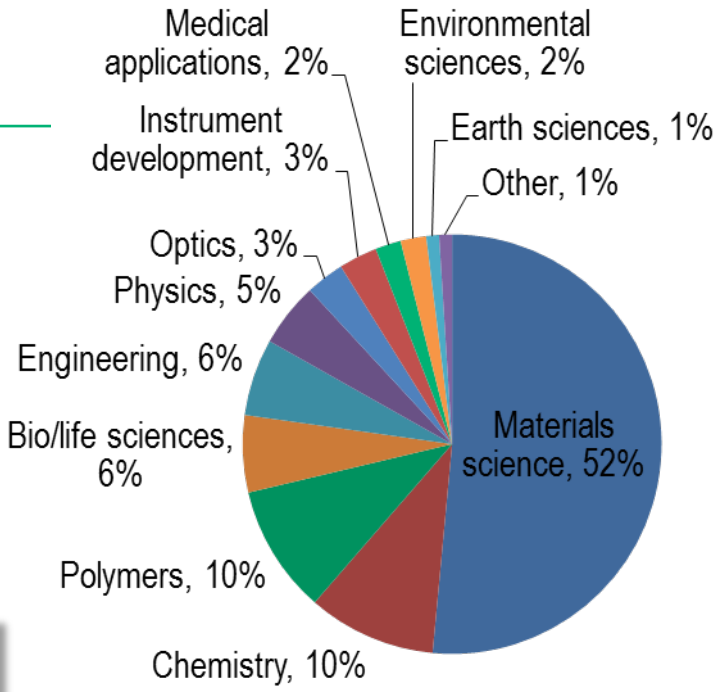
Center for Nanophase Materials Sciences:
A synergistic user and science facility

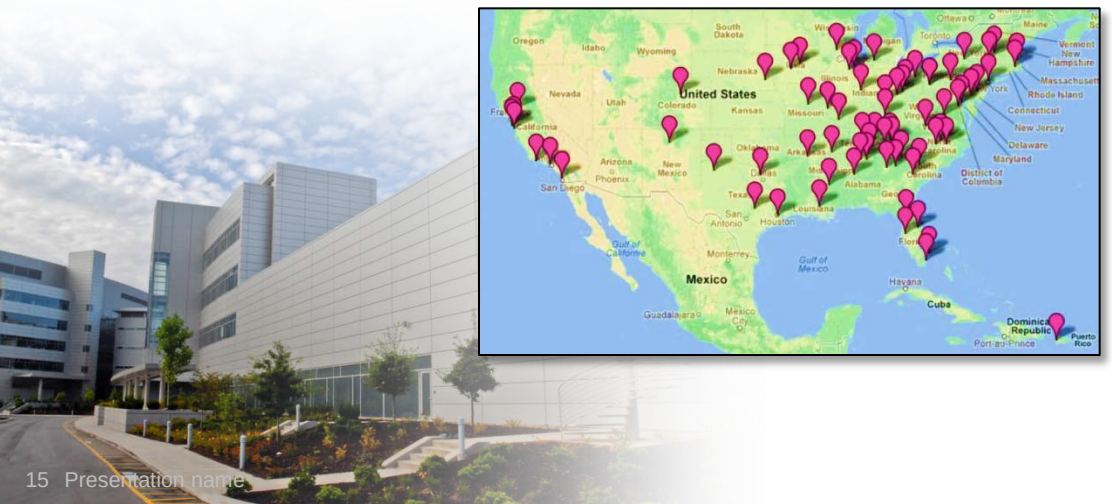
Synergizing and amplifying ORNL signature strengths

- Neutron science
- High-performance computing
- Materials and chemistry
- Microscopy

3 major research themes

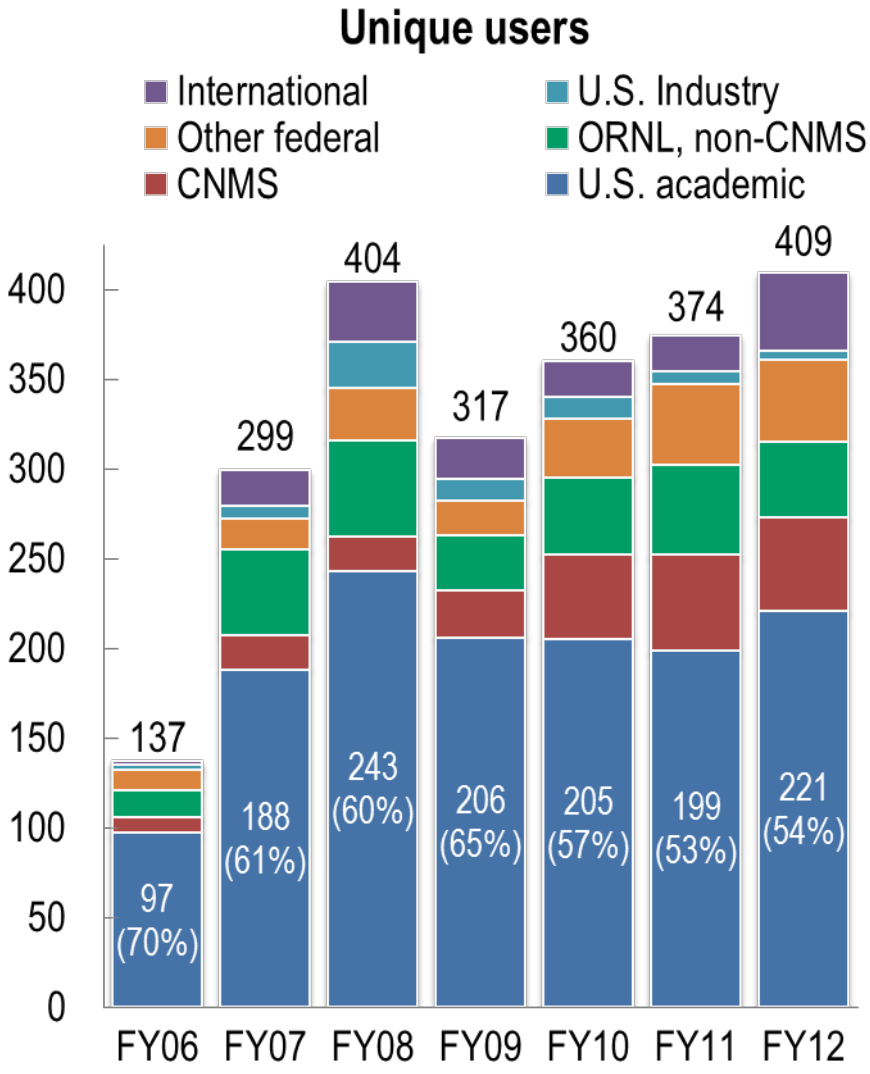
- Electronic and ionic functionality on the nanoscale
- Functional polymer and hybrid architectures
- Collective phenomena in nanophases

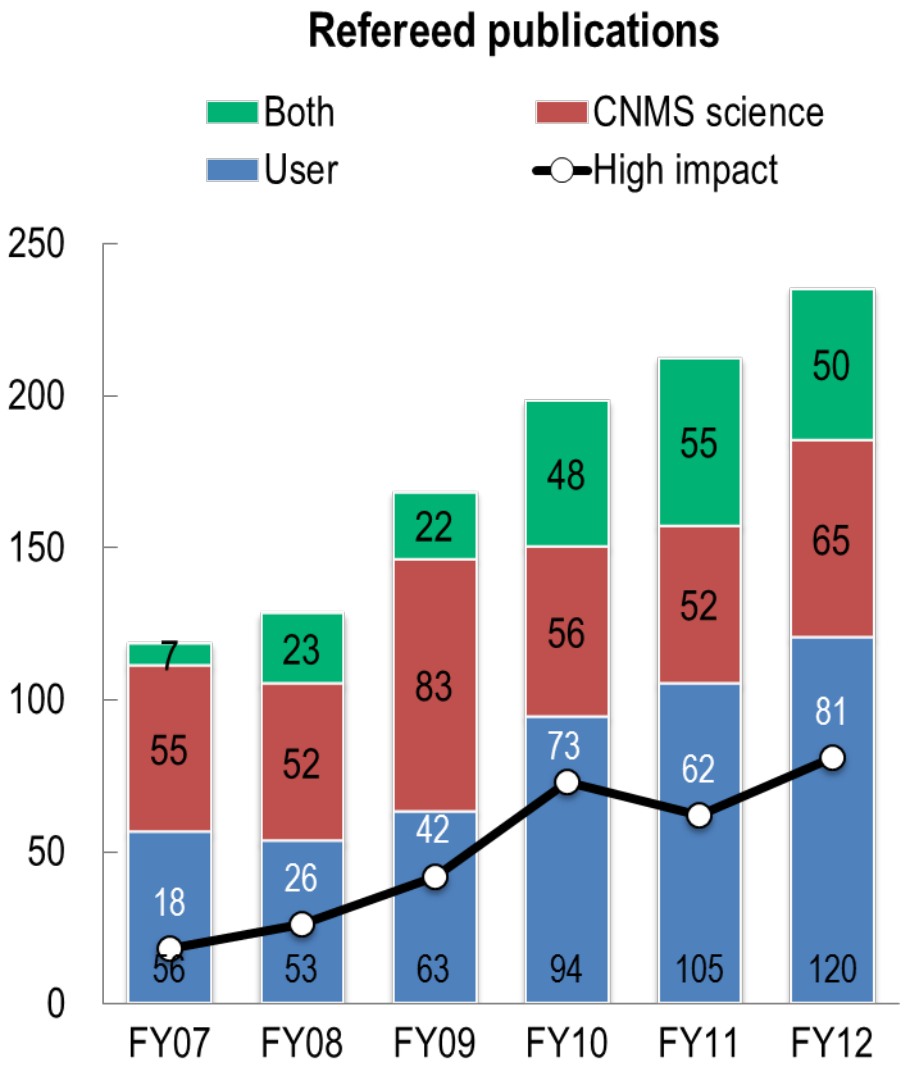




Supporting a diverse user base with forefront equipment and expertise

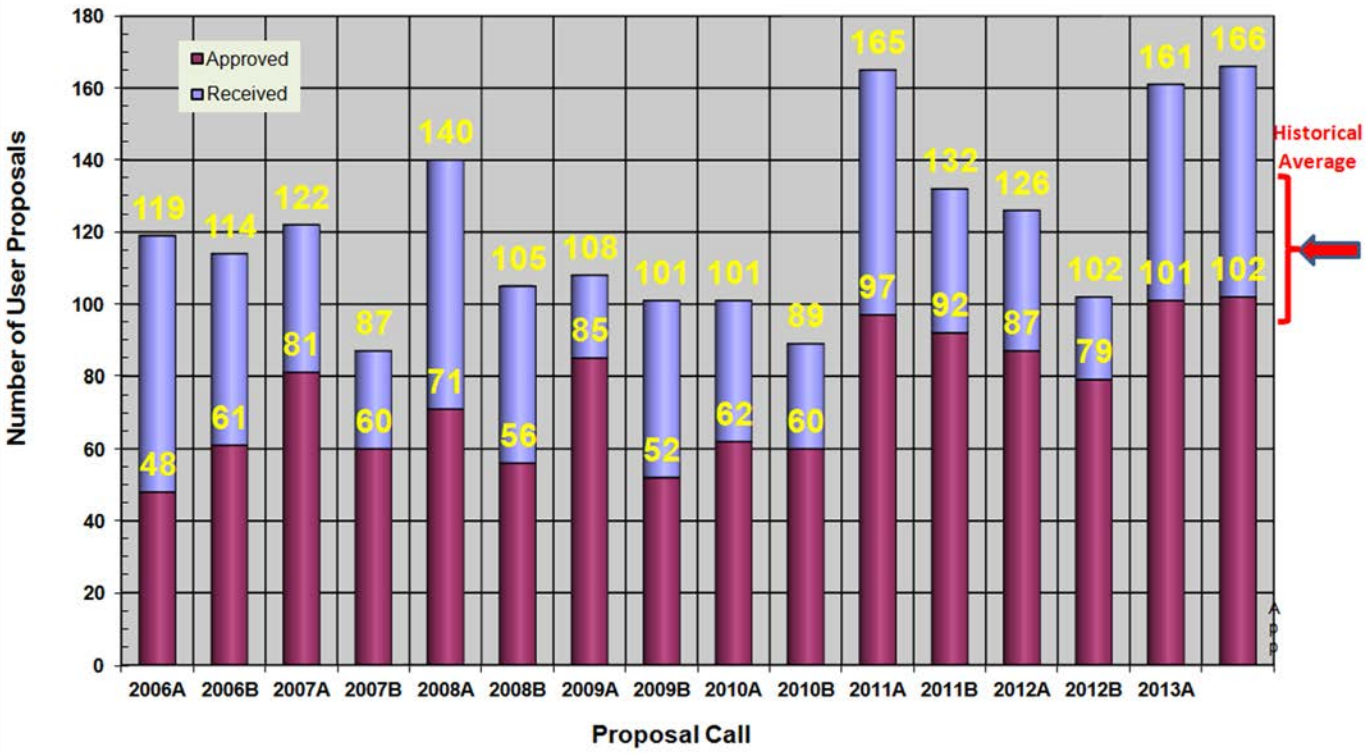
Center for Nanophase Materials Sciences
Enabling advances in nanoscience





User Program

- **User Proposal Call 2013B**
  - **166 proposals received for May 1 deadline- new record for CNMS**
  - **102 proposals approved last Friday, June 21 (61%)**



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Theme 1: Electronic and ionic functionality on the nanoscale

Goal

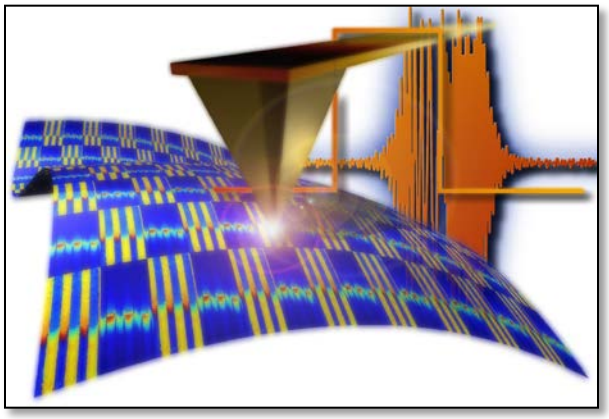
Understand behaviors of electronic and ionic materials at the scales of defects, nanostructures, and microdevices

Signature strengths

- Scanning probe microscopy
- Nano-enabled electrochemical catalysis

Scientific impacts

- Electronic transport and phonon functionality
- Nanoscale electrochemistry and ionics
- New catalytic routes to functional energy materials
- Energy conversion and storage



Band excitation technique
in scanning probe microscopy

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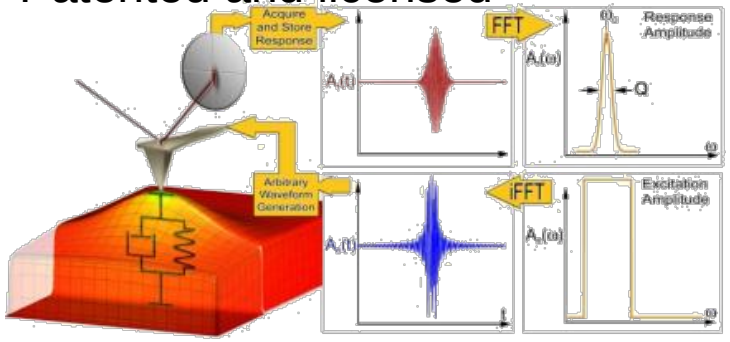
Fundamental imaging science advances have led to new characterization tools

Band excitation

- Introduction of **parallel** frequency detection:
  - Fully captures tip-surface interactions
  - Allows ~100 increase in S/N ratio by resonance enhancement
  - Directly measures energy dissipation
- 50+ research papers (>25 high profile)
- Patented and licensed

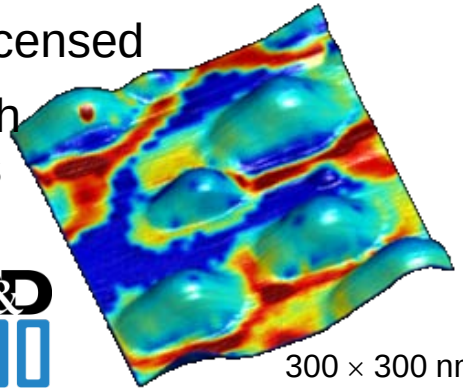


Driving with a band of frequencies yields a full system response

Jesse, Kalinin et al., *Nanotechnol.* **18**, 435503 (2007)

Electrochemical strain microscopy

- Electrochemical reactivity and ionic transport in solids at <10 nm scales
- Detection of picometer strains induced by ion motion
  - Li-ion solid electrolytes, cathodes, and anodes
  - Fuel cell cathodes
  - Memristive and electroresistive switching
- Patented and licensed
- Recognized with multiple awards



Balke et al., *Nature Nanotechnol.* **5**, 749−754 (2010)

Theme 2: Functional polymer and hybrid architectures

Goal

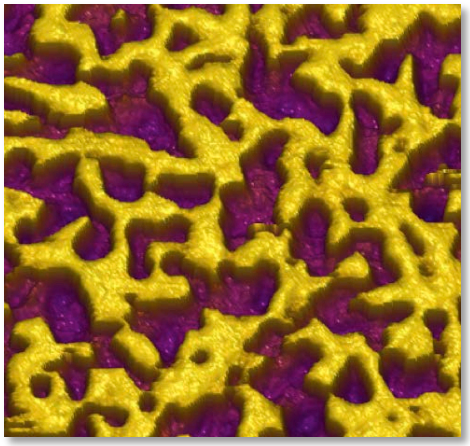
Understand and control the multiscale organization of conformationally asymmetric macromolecular and hybrid nanomaterials, to achieve functionality capable of capturing, transporting, and transforming energy

Signature strengths

- Macromolecular synthesis, characterization, and separation
- Selective deuteration
- Neutron and optical studies of structure, dynamics, and functionality

Scientific impacts

- Organic electronic energy materials
- Soft and hybrid materials by design
- Multiscale functional structures



AFM image of P3HT-b-PFO conducting block copolymer

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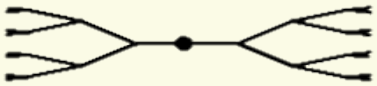
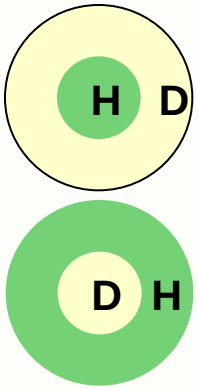
Deuteration and neutron scattering
Resolving the debate on solvated structure of dendrimers

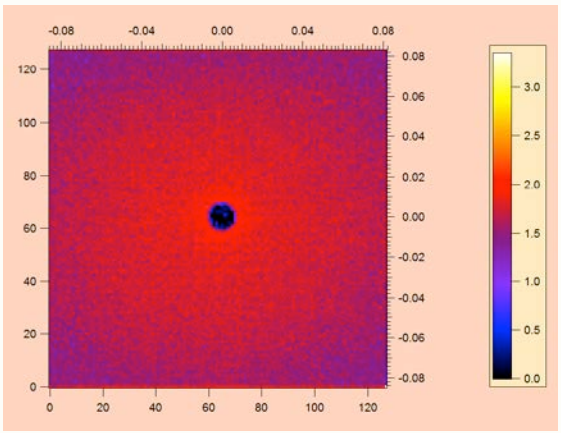


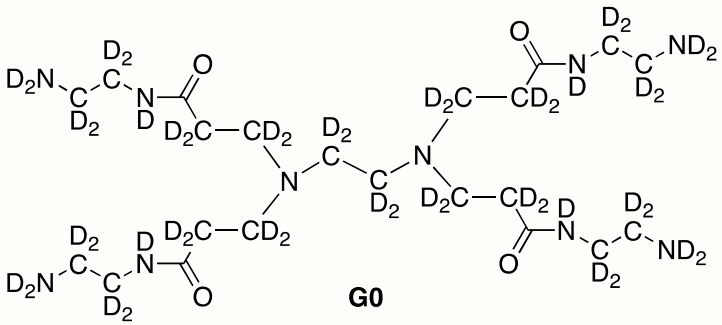
de Gennes et al., 1983:
Dense shell

Current theory supports the dense-core model, but no convincing experimental evidence, Likos et al., 2006

Muthukumar et al., 1990:
Dense core







Structure of deuterated G0 PAMAM

Wu et al., 2011: SANS from selectively deuterated G5 PAMAM dendrimers proves segmental backfolding (dense core) **unambiguously** (*J. Chem. Phys.* 135, 144903)

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Theme 3: Collective phenomena in nanophases

Goal

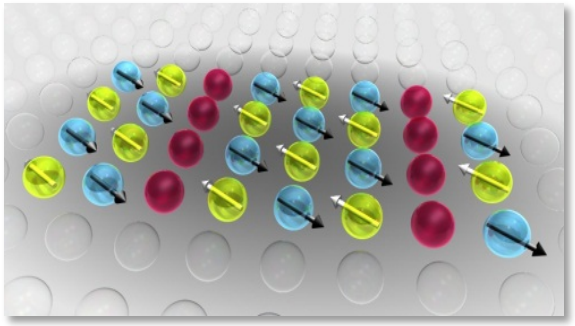
Understand collective phenomena that arise from fluctuations, nanoscale confinement, and integration across length and time scales; and control these phenomena to produce complex functionality

Signature strengths

- Theory and methods for strongly correlated electronic materials
- Soft matter simulations
- Nanofabrication and nanofluidics
- Bio-inspired nanoscience

Scientific impacts

- Innovations in nano-bio science and technology
- Strongly correlated and low-dimensional materials
- Multifunctional materials discovery and design



Simulation of 2D Hubbard model with nanoscale charge stripes

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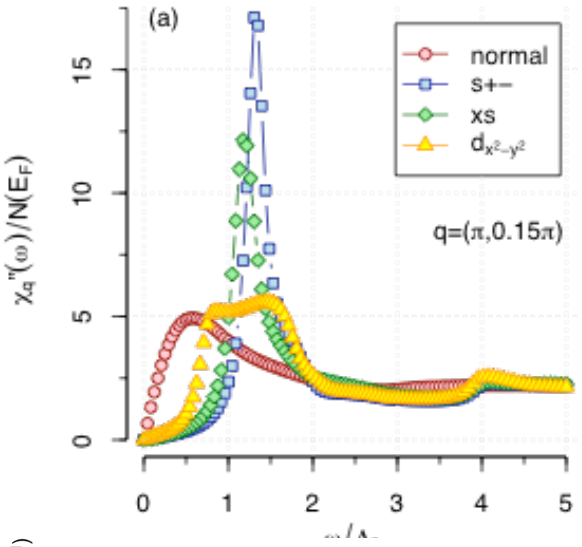
Understanding and predicting high-T_c superconductivity

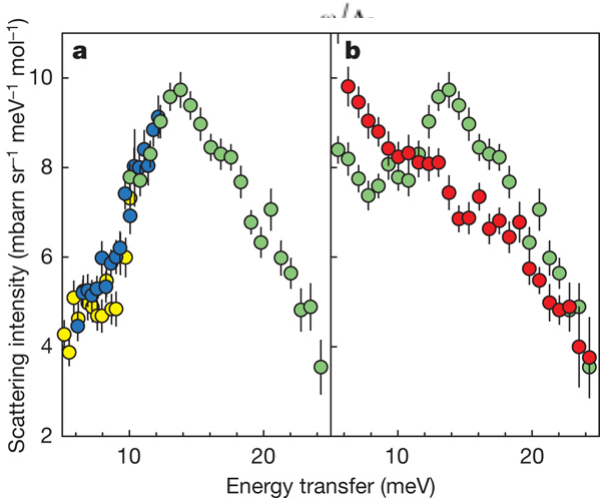
Building the scientific foundation for a wide range of energy-relevant technologies

- **Nanoscale stripe inhomogeneities in cuprates reveal enhanced superconductivity**
- **Prediction of neutron resonance in Fe-based superconductors**
- **Prediction of higher-T_c superconductivity in bilayer systems**
- **2008 Gordon Bell award: First petascale application**
- **22 publications on Fe systems over past 5 years**



Theoretical prediction of neutron resonance

T. A. Maier (CNMS) and D. J. Scalapino (UCSB), 2008–2009

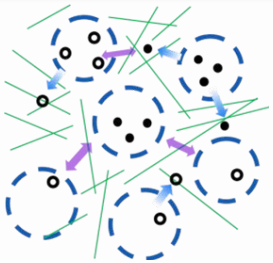


Experimental verification

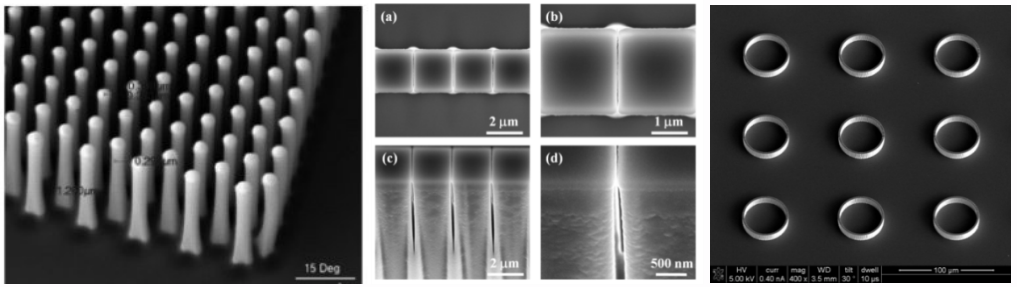
A.D. Christianson et al., *Nature* 456, 930 (2008)

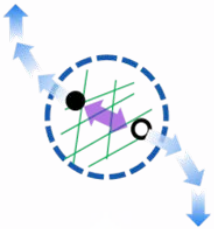
M. D. Lumsden et al., *Phys. Rev. Lett.* 102, 107005 (2009)

Collective phenomena from the bottom up

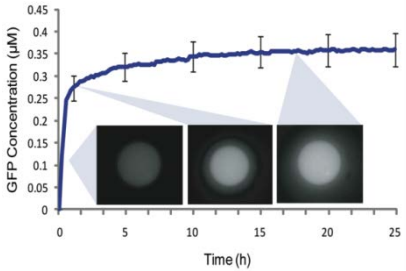


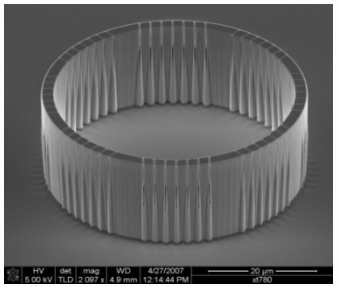
Communication between elements of hierarchical systems coordinates function



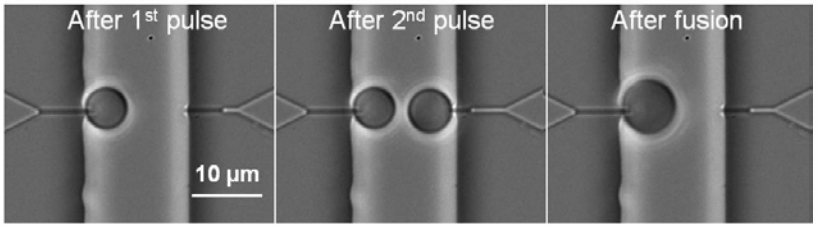


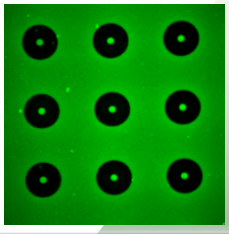
Exchange of energy, information and materials between reaction systems and their environment can be controlled using nanostructured materials





Crowding in chemical reaction systems can be controlled using advanced nanofluidic and fabrication techniques





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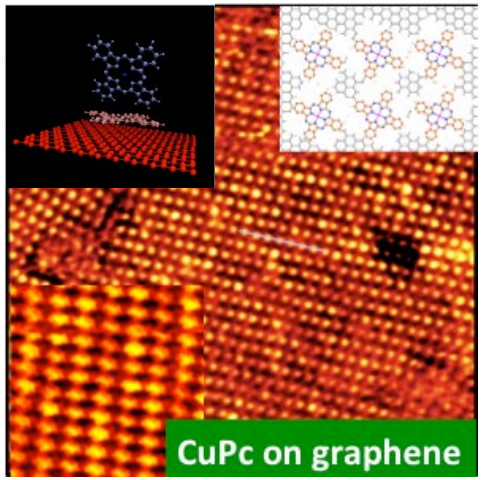
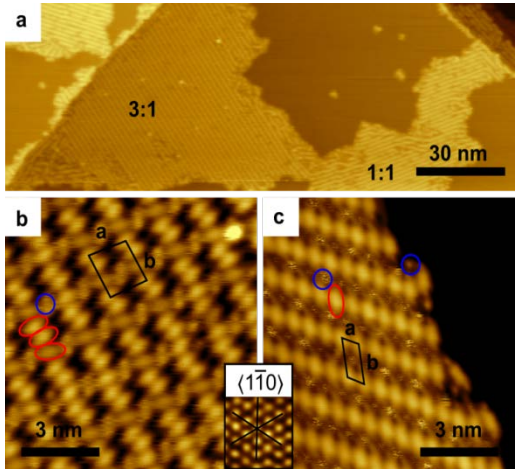
2D Semiconductor Nanomembranes: *Moving Beyond Graphene*

Surface-induced orientation control for growth of organic crystals on graphene



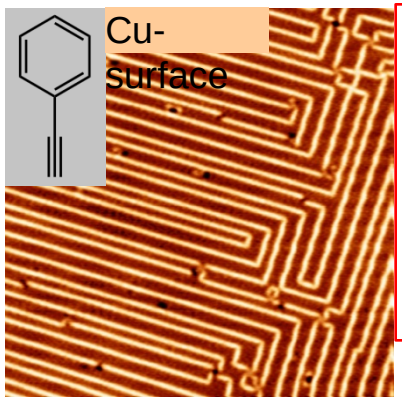
K. Xiao, D. Geohegan, *et al., J. Am. Chem. Soc.* (2013)

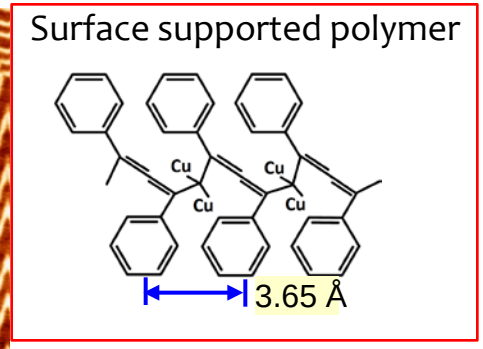
Controling charge-transfer salts down to molecular building blocks: direct imaging of cations and anions



P. Maksymovych, B. Sumpter et al

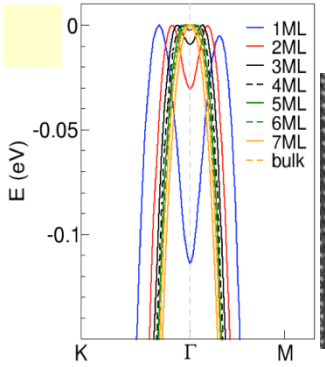
Unique surface-assisted polymerization

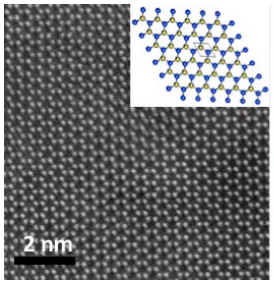


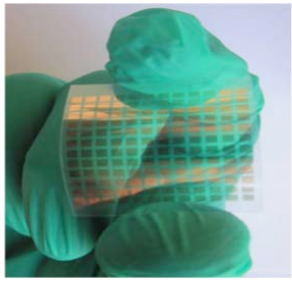


Minghu Pan *et al*

Highly Responsive Ultrathin GaS Nanosheet Photodetectors on Rigid and Flexible Substrates







M. Yoon, K. Xiao, et. al.

Highly promising next generation materials

BES Triennial Onsite Review
Sept 24-26th, 2013

- **Three theme documents; plus facility overview document**
- **Integration with laboratory – neutrons; computing; materials**
- **Five year outlook.**

Smith (CNMS Director)

Zetans (Division Admin Assistant)

Liaison:
Rondinone* (Industry)
Hong* (Neutron Science)

Theme Leads:
Kalinin* (Electronic and Ionic Functionality on the Nanoscale)
Sumpter* (Functional Polymer and Hybrid Architectures)
Simpson* (Collective Phenomena in Nanophases)

Managers:
Tony Haynes (User Program)
Lowe (User Prog Admin)
Scott Hollenbeck (ESH& Ops)
Goins* (Ops Support)
Taylor (Env Protection)

NanoFabrication

- **Simpson*** (Group Lead)
  Garner (Group Admin)
- Retterer
- Collier
- Lavrik
- Doktycz
- Fowlkes
- Kravchenko
- Rack
- **Briggs** (nanofab task lead)
- Hensley
- Lester
- Srijanto

Imaging and Nanoscale Characterization

- **Baddorf** (Group Lead)
  Goins* (Group Admin)
- Kalinin*
- David Joy
- Li
- Jesse
- Tselev
- Balke
- Maksymovych
- Pan
- Gai
- Ivanov*

Electron Microscopy

- **More** (Group Lead)
- Idrobo
- Chi
- Unocic
- Powers
- Jihua Chen
- Miller

Nanomaterials Theory Institute

- **Sumpter*** (Group Lead)
  Lohman (Group Admin)
- Kent
- Maier
- Smith*
- Cummings+
- Zhang
- Beste
- Alvarez-Compot
- Fuentes-Cabrera
- Cook+
- Ganesh
- Goswami
- Huang
- Jakowski
- Kumar
- Reuter
- Yoon

Nanoscale Synthesis and Functional Assembly

- **Geohegan** (Group Lead)
  Holbrook (Group Admin)
- Ivanov*
- Xiao
- Puretzky
- Rouleau
- Fleming
- **polymer task lead** (vacant)
- Pickle
- Hong*
- Lokitz
- Uhrig
- Kilbey
- Bonnesen
- Messman
- **Rondinone*** (Catalysis task Lead)
- Liang
- Biegalski
- Dai
- Overbury
- Wu
- Schwarz
- Pawel
- Keum

Integration with Electron Microscopy User Facility (ShaRE): 1st Oct 1013

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