Nanoscale Science Research Centers (NSRCs): Impact and Future Directions

Report to BESAC by Co-Chairs

Murray Gibson, Florida A&M University-Florida State University

Karl Mueller, Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY

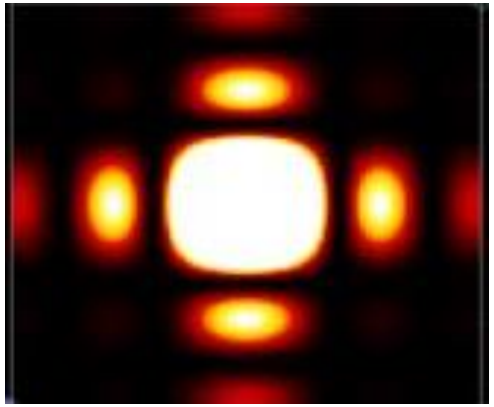
Outline

Charge to NSRC Sub-Committee

Overview of NSRC Research Centers

Findings and Recommendations

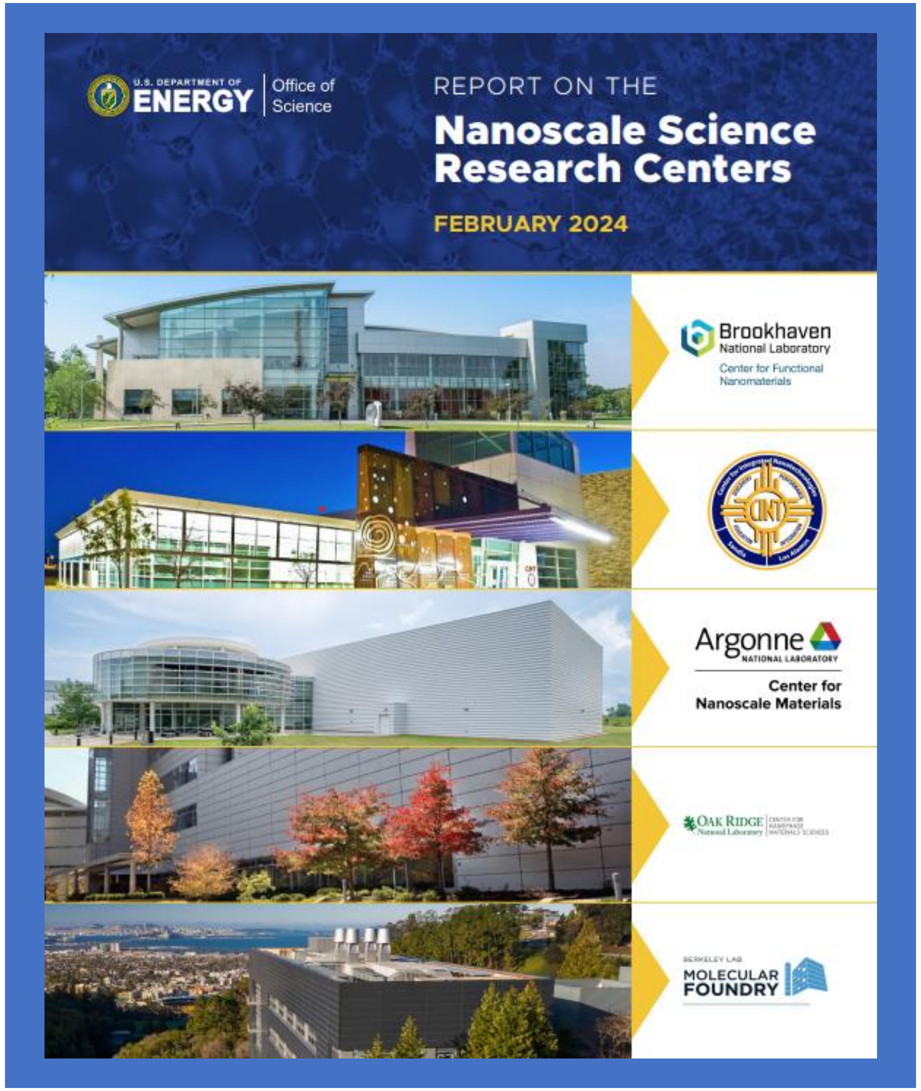
Executive Summary



Charge to NSRC Sub-Committee

Provide Strategies for selecting high-impact, future directions for NSRCs that considers:

- What has been the impact of the NSRCs?
- How are the collective NSRCs synergistic?
- NSRC synergies with the other user facilities at the laboratory?
- Best practices and opportunities for diversifying the user community?
- How should the NSRCs evolve to better serve the nation and user research?



NSRC Committee Members

Co-Chairs

- J. Murray Gibson, FAMU-FSU
- Karl Mueller, PNNL

Subcommittee Members

- Harry Atwater, Caltech
- Donna Chen, University of South Carolina
- Yi Cui, Stanford University
- Abhaya Datye, University of New Mexico
- Helmut Dosch, DESY
- Yan Gao, GE (retired)
- Clare Grey, University of Cambridge
- Sossina Haile, Northwestern University
- Boris Kozinsky, Harvard University
- Abbas Ourmazd, University of Wisconsin, Milwaukee
- Joan Redwing, Pennsylvania State University
- Frances Ross, MIT
- Eric Stach, University of Pennsylvania
- Cathy Tway, Johnson Matthey

Office of Basic Energy Sciences Participants

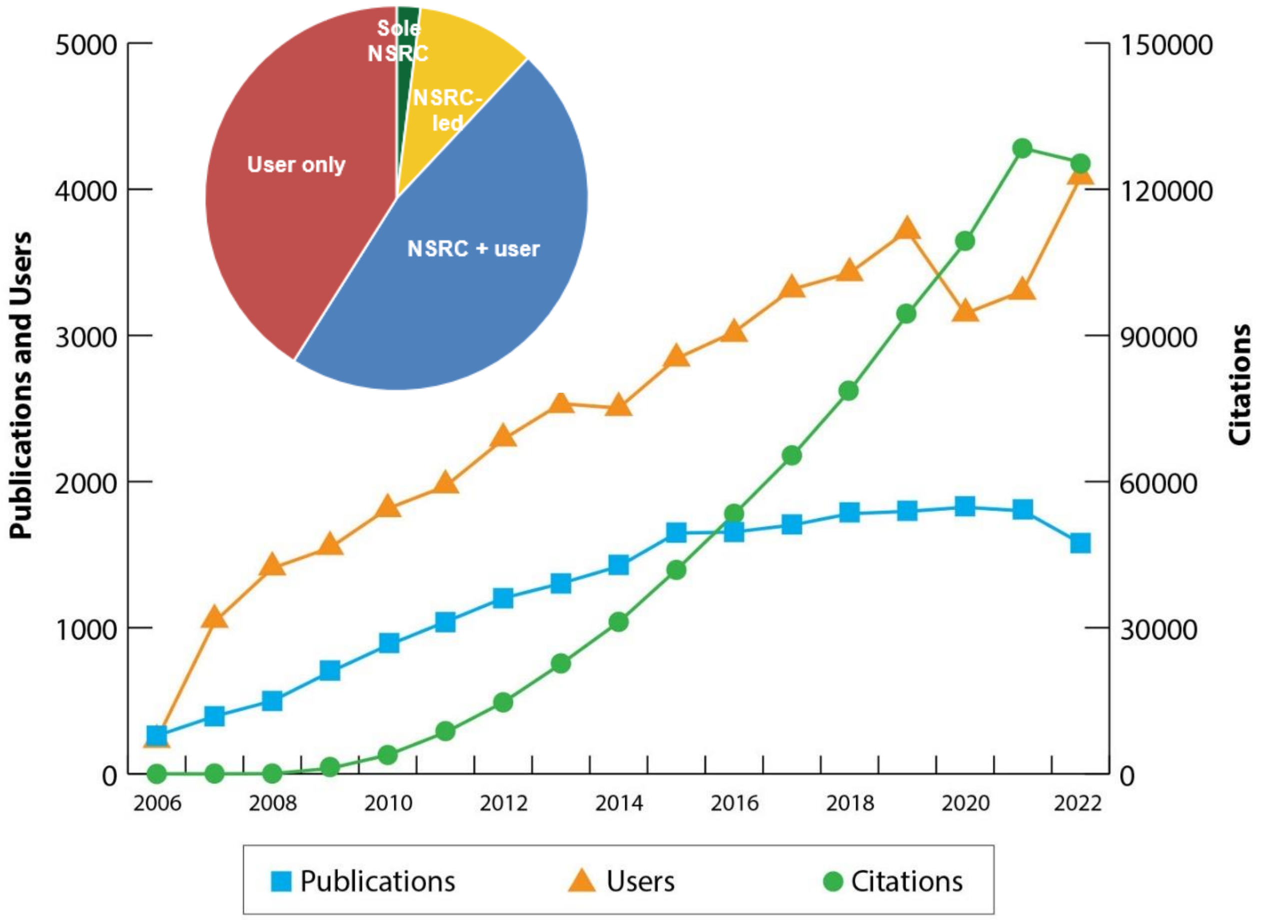
- Linda Horton
- Andrew Schwartz
- Gail McLean
- Adam Kinney
- Dava Keavney
- Mikhail Zhernenkov
- Kerry Hochberger

Selected Capabilities and Strategies

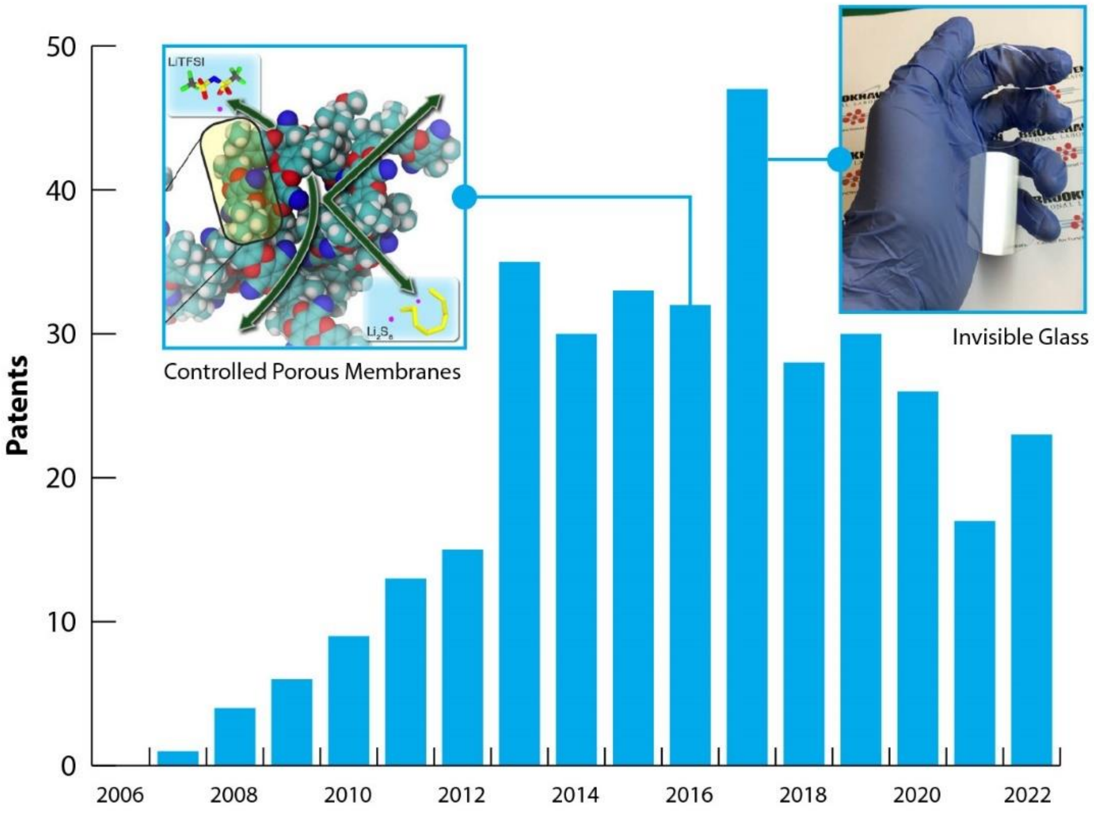
NSRC	CFN	CINT	CNM	CNMS	Foundry
					
Specialized Capabilities	In situ and operando X-ray and electron microscopy and spectroscopy	Microelectronics and quantum device fabrication	Hard X-ray nanoprobe beamline	Automated flow reactor for polymer synthesis and site-specific deuteration	Terahertz scanning tunneling microscope/ atomic force microscope
Strategic Directions	Autonomous nanomaterials discovery	Quantum materials systems	Nanoscale discovery for sustainable energy	Soft matter science	Big data electron microscopy
Overlapping	electron microscopy | nanofabrication | computing resources | theory and modeling				

Impact by the Numbers

Publications

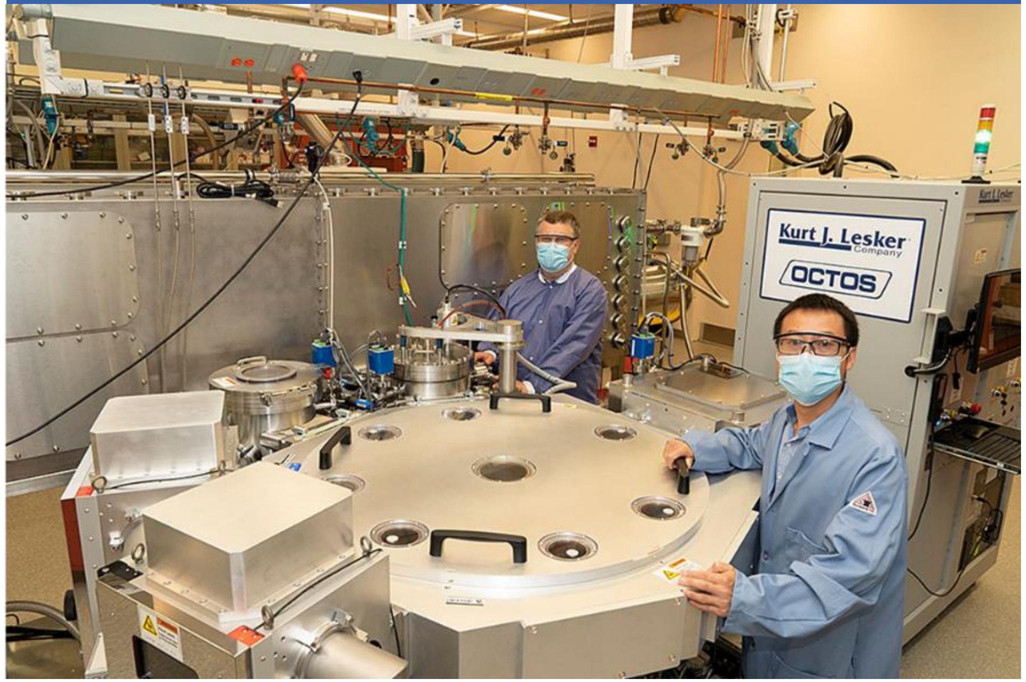


Patents



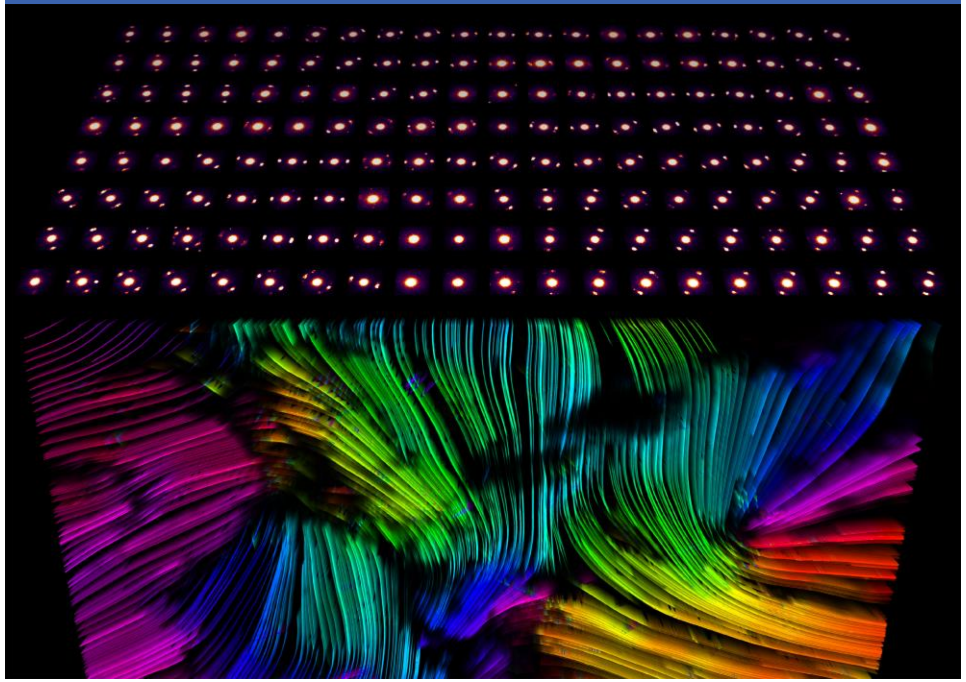
Innovating Instrumentation

Quantum Materials Factory



Q-Press at CFN

4-D STEM



Scanning Transmission Electron Microscopy at MF

Instrument-Savvy People

NREL

Katherine Jungjohann

Berkeley

Jeffrey Neaton

U. Puerto Rico

Armando Rúa

ORNL

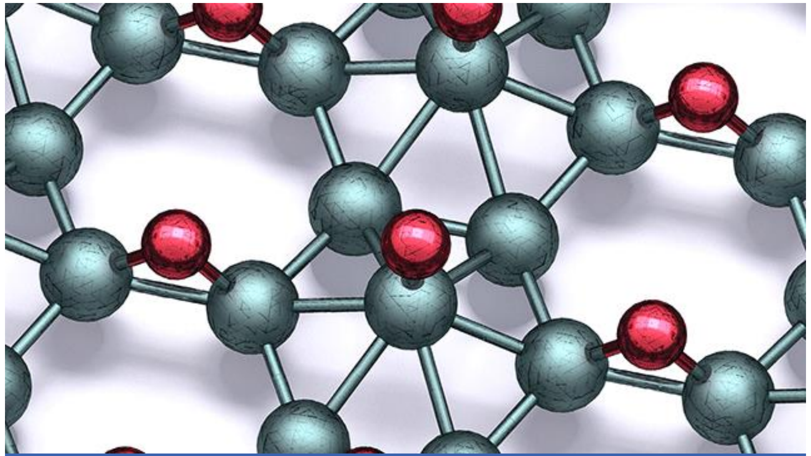
Rama Vasudevan

Heidelberg

Jana Zaumseil

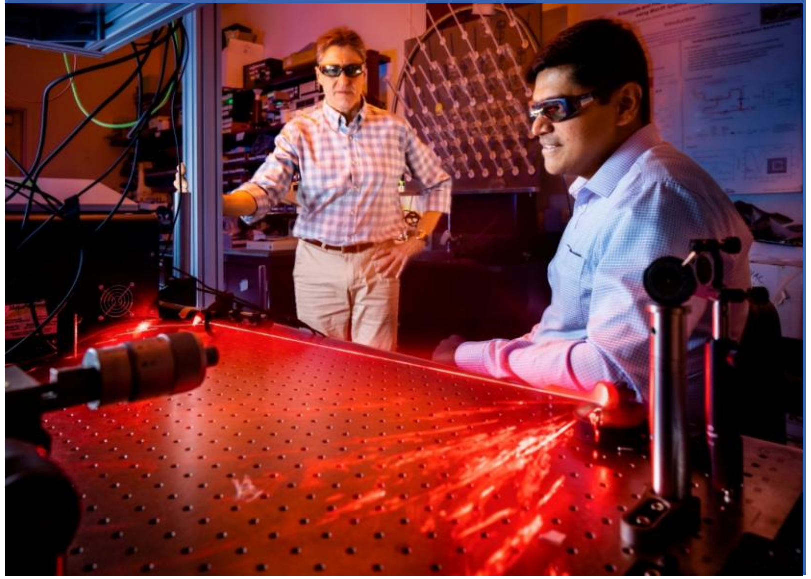
Former postdocs, staff, and users have taken leadership roles around the world

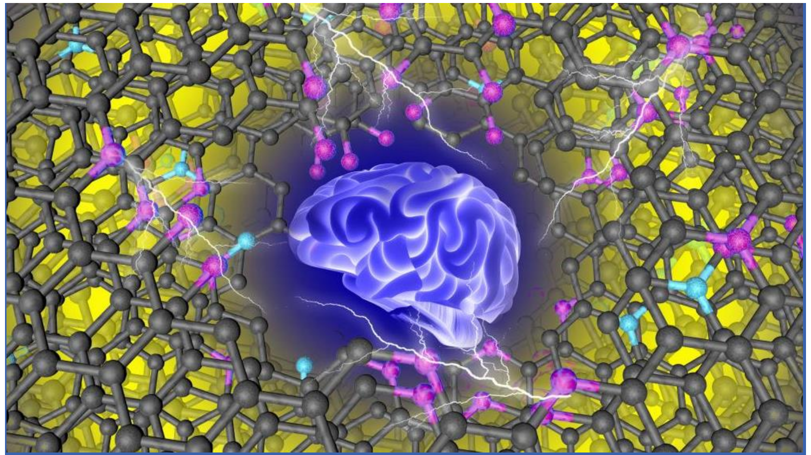
Impactful Science



Borophane – a new stable 2D material
Science 371, 1143 (2021)
CNM

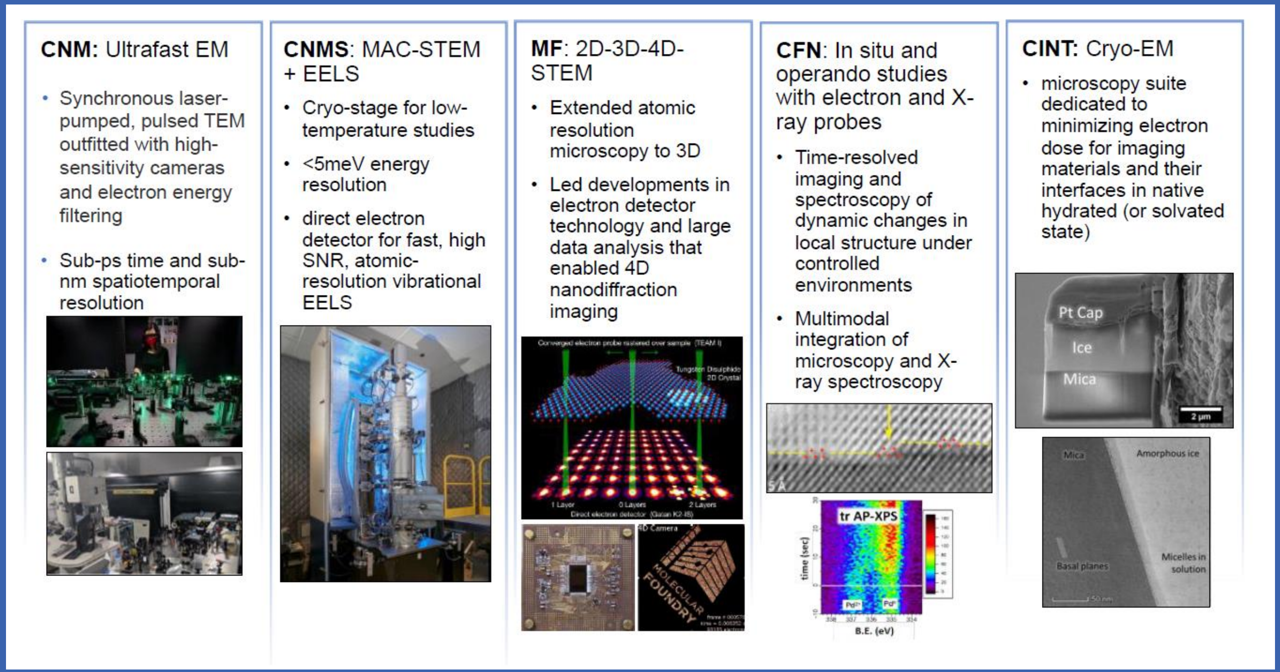
Ultrafast light steering with metamaterials
Nature Photonics 17, 588-593 (2023)
CINT





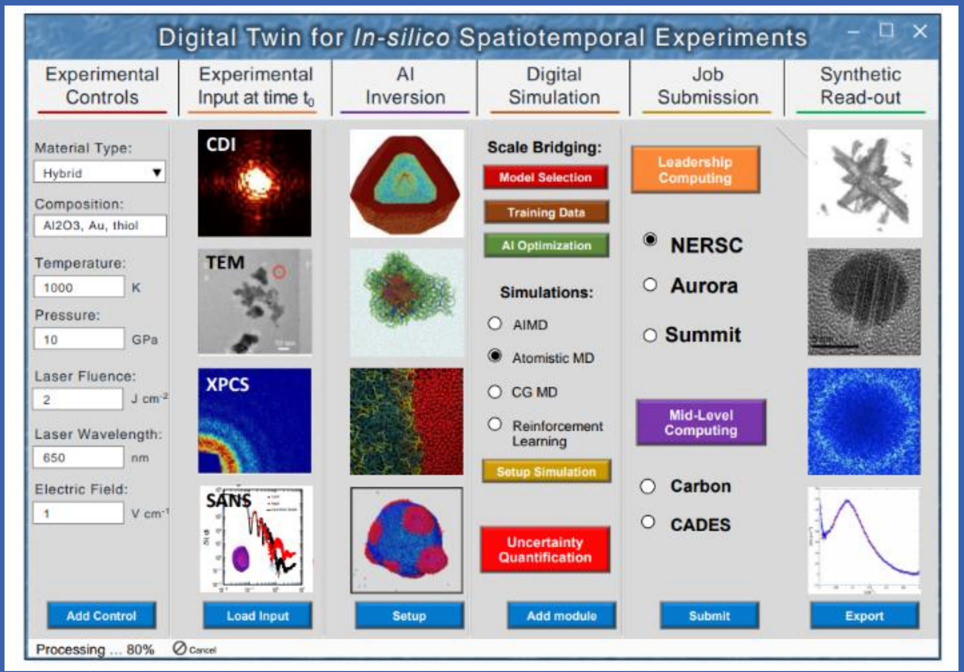
Better supercapacitors thanks to machine learning
Nature Communications, **14,** 4607 (2023)
CNMS

Working Together



Complementary TEM developments

In this area, centers are distinctive and complementary

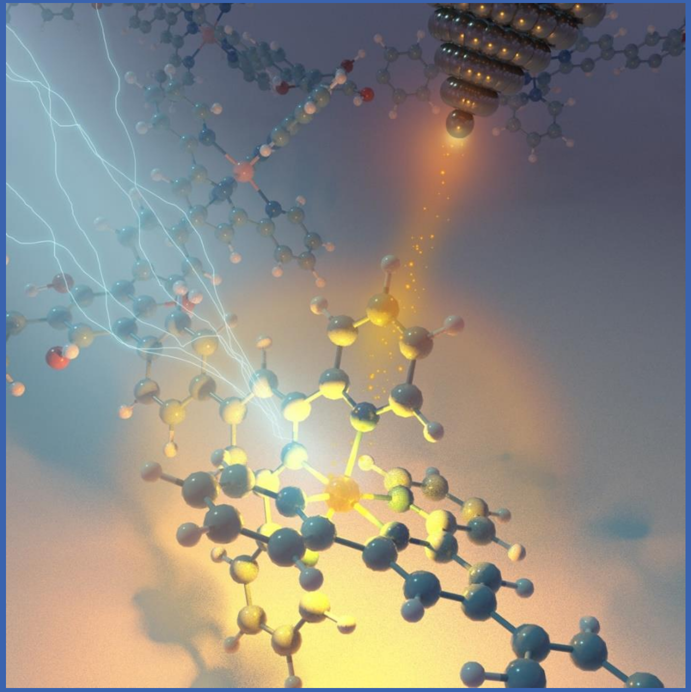


Collaboration across scientific user facilities

CNM, CNMS, MF, CFN, CINT, APS, ALS, SLAC

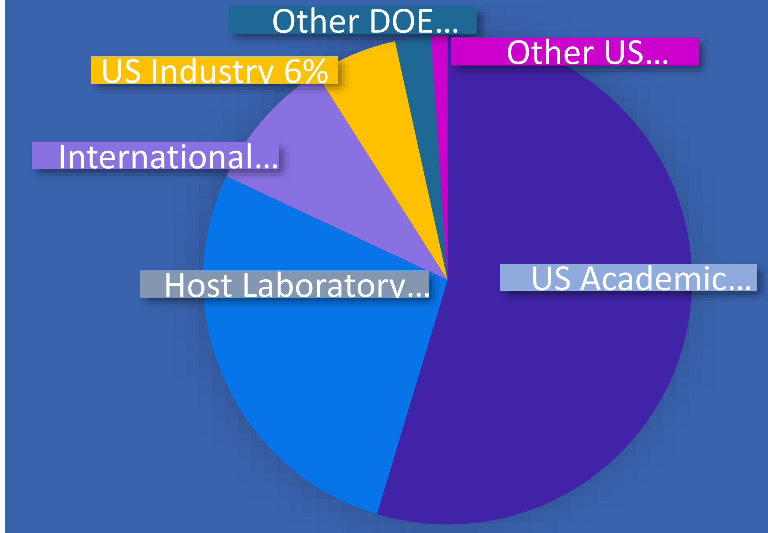
Exciting future ideas in Instrument Automation, AI/ML and Data

Leveraging Partner User Facilities



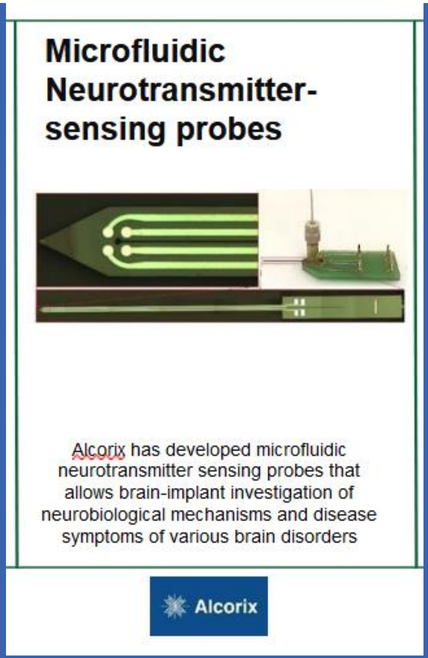
A single atom – chemically characterized by x-ray spectroscopy for the first time *Nature,* **618,** 69-73 (2023) **CNM/APS**

Broadening the User Base



Good institutional diversity but need to attract non-R1 university users

Increasing outreach to diversify the user community



CNM/ANL Spinoff

Industrial work by small companies and instrument manufacturers is strong. Large companies need more attention

Summary of NSRC Impacts

- First NSRC opened its doors for user research about 20 years ago (2006)
- Five NSRCs now serve over 4,000 users annually
- Spanned a broad range of research topics, bridging synthesis/fabrication, characterization, and theory/modeling/computational/data science
- Evolved from a new methodology to an established foundational capability for science and commercial technologies
- Expanded capabilities to include the electron microscopy user facilities and quantum information sciences
- Played a signature role in advancing science and supporting innovations in instrumentation and techniques for nanoscience research
- Provided a distinctive source of trained scientists and engineers
- Provided critical tools for advancing today's science and technology grand challenges
- Complimented investments from other agencies and build expertise of DOE user facilities

The NSRCs have made major positive impacts on materials and nanoscience research in the United States and beyond.

High-Level Recommendation

The nation should **sustain and strengthen** the collection of NSRCs that has become a key element of US competitiveness for research on high priority scientific problems and in instrumentation development.

Center for Nanoscale Materials
Argonne National Laboratory

Molecular Foundry
Lawrence Berkeley National Laboratory

Center for Functional Nanomaterials
Brookhaven National Laboratory

Center for Integrated Nanotechnologies
Sandia National Laboratories
Los Alamos National Laboratory

Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

Findings and Recommendations

The NSRCs are a valuable and innovative national asset that contribute multiple critical capabilities and steward scientific excellence in key areas. We recommend that the nation sustain and strengthen the NSRC ecosystem that has become a key element of US competitiveness for high priority scientific problems and in instrumentation development.

Findings and Recommendations

The NSRCs are a valuable and innovative national asset that contribute multiple critical capabilities and steward scientific excellence in key areas. We recommend that the nation sustain and strengthen the NSRC ecosystem that has become a key element of US competitiveness for high priority scientific problems and in instrumentation development.
Success lies in the exceptional combination of instrumentation and in-house expertise made available to many thousands of users. The NSRCs also train many instrumentation-aware scientists and engineers, fulfilling a recognized deficit in US competitiveness.
While the centers were created to address the needs of nanoscience and technology, the centers—and the field itself—have become integrated into almost every area of contemporary science and engineering research. The NSRCs are playing an increasingly important role in national priority areas such as energy, microelectronics, biotechnology, quantum information science, advanced manufacturing, high performance computing, artificial intelligence, and autonomous systems.

Findings and Recommendations

Individually, the NSRCs have provided sustained impact in the fields allied with nanotechnology. Together, these strengths could be combined for constructive impacts that will far outweigh the individual efforts. We recommend that the NSRCs develop a singular strategic plan involving all five centers, focusing on national science priorities and grand challenge areas. The broad expertise of the NSRCs, in its totality, represents a leading force that can help the US regain international leadership in instrumentation-enabled science.

Findings and Recommendations

Individually, the NSRCs have provided sustained impact in the fields allied with nanotechnology. Together, these strengths could be combined for constructive impacts that will far outweigh the individual efforts. We recommend that the NSRCs develop a singular strategic plan involving all five centers, focusing on national science priorities and grand challenge areas. The broad expertise of the NSRCs, in its totality, represents a leading force that can help the US regain international leadership in instrumentation-enabled science.

Take advantage of opportunities to work collectively and provide leadership internationally and in research for priority scientific areas for the nation.
Ensure engagement with the broader community of scientists and prioritize efforts, especially collaborative efforts among NSRCs, in the co-development of science-driven novel instrumentation and an infrastructure that provides for management and analysis of ever-increasing amounts of scientific data and metadata.
Simplify the process for users through a single portal for user proposals. and challenge the user community to generate proposals that take advantage of multiple facilities and develop mechanisms that promote multi-facility utilization.
Continue advances in remote access capabilities that were established during the COVID-19 pandemic, which could also increase engagement of non-R1 MSIs and ERIs in the user community.

Findings and Recommendations

The impact of the focus on instrumentation and training of instrumentation-aware staff is clear based on the impacts of the NSRCs. We recommend an increase in the training of instrument-knowledgeable scientists and engineers through expanded postdoc programs at the NSRCs.

Findings and Recommendations

The impact of the focus on instrumentation and training of instrumentation-aware staff is clear based on the impacts of the NSRCs. We recommend an increase in the training of instrument-knowledgeable scientists and engineers through expanded postdoc programs at the NSRCs.

Many former NSRC staff and postdocs have moved into research and academic positions elsewhere. This valuable trend builds the user community and leverages the US science and technology enterprise.

Success in this area will enhance the necessary expertise to launch and realize future strategic science directions and increase the leveraging of the user program by enabling staff scientists to expand their user collaborations.

Findings and Recommendations

The decision to co-locate the NSRCs with other DOE capabilities was a prescient strategy that has resulted in a major strength of the collected capabilities. We recommend that the NSRCs take full advantage of the increased capabilities that will be afforded by current and planned large facility upgrade projects (x-ray light and neutron sources, high performance computing and networking).

Findings and Recommendations

The decision to co-locate the NSRCs with other DOE capabilities was a prescient strategy that has resulted in a major strength of the collected capabilities. We recommend that the NSRCs take full advantage of the increased capabilities that will be afforded by current and planned large facility upgrade projects (x-ray light and neutron sources, high performance computing and networking).
The co-location of each NSRC with unique large-scale facilities such as x-ray and neutron sources has been one of the important elements of their success.
The NSRCs should work with their partner scientific user facilities and leadership-class computing facilities to take advantage of upgrades and new capabilities, and this includes but is not limited to co-developed capabilities and beamlines.

Findings and Recommendations

On-going emphasis of the Centers on broad outreach is critical for increasing impact and the elevation of science and technology from historically under-represented groups. We recommend that the Centers focus on considerable expansion of their proactive efforts to increase the diversity of their user community and their staff.

Findings and Recommendations

On-going emphasis of the Centers on broad outreach is critical for increasing impact and the elevation of science and technology from historically under-represented groups. We recommend that the Centers focus on considerable expansion of their proactive efforts to increase the diversity of their user community and their staff.

While their recent efforts to increase outreach to new user communities will be effective, they should expand their emphasis on training, such as through summer schools and short courses, to reduce the barrier to entry for new users and increase interest in the centers as a career opportunity for a broader set of scientists and engineers.

Findings and Recommendations

The Centers have experienced good but limited success in industrial interactions that represent a growing opportunity in areas such as microelectronics and quantum information science. We recommend increased efforts to lower barriers to industry participation and enhance industrial interactions with NSRC staff.

Findings and Recommendations

The Centers have experienced good but limited success in industrial interactions that represent a growing opportunity in areas such as microelectronics and quantum information science. We recommend increased efforts to lower barriers to industry participation and enhance industrial interactions with NSRC staff.
The NSRCs have a history of excellent collaborations and partnerships with instrumentation development companies. They have also been very effective in connecting with small companies associated with technology spinoffs, and this is very valuable to regional economic growth. However, their engagement with larger companies has been relatively limited.
They should continue efforts that encourage meaningful engagement with industry on relevant science challenges. More extensive interactions with industry beyond the user program, e.g., through affiliates, focused short courses, and invited seminars, would be valuable.

Executive Summary (Part 1)

- The subcommittee **affirms** that the **NSRCs have made major positive impacts on materials and nanoscience research** in the United States and beyond.
  - Play a signature role in **advancing science and supporting innovations in instrumentation and techniques** for nanoscience research.
  - Provide a distinctive **source of trained scientists and engineers**.
  - Provide **tools that are critical for advances** in most of today's science and technology grand challenge areas, including microelectronics, energy, biotechnology, quantum information science, advanced manufacturing, high performance computing, artificial intelligence, and autonomous systems.
  - **Complement investments from other agencies**, such as the National Science Foundation, to build on DOE Office of Science expertise in user facilities for the service of a broad science and user community.

Executive Summary (Part 2)

- **Recommendations** chart a **pathway to accelerate the impact of the centers** in the coming years, rising to the challenge of **addressing emerging priorities and critical needs** for US competitiveness.
  - **Sustain and strengthen the NSRCs** that has become a key element of US competitiveness research on high priority scientific problems and in instrumentation development.
  - Increase the inventory of **world-leading instruments and experts** to support a **growing user community**.
  - **Work co-operatively and synergistically** in addressing national grand challenges, with **strategies developed in concert with BES and the user community**. Efforts to synergize so far have been very successful and should be greatly amplified.
  - **Expand postdoctoral training programs** across the NSRCs, as well as a **broaden the user communities** to address the human capital needs of the nation.
  - **Leverage the ongoing upgrades of large facilities,** such as x-ray and neutron sources

Questions?

Murray Gibson, Florida A&M University-Florida State University

Karl Mueller, Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY