U.S. DEPARTMENT OF ENERGY | Office of Science

REPORT ON THE

Nanoscale Science Research Centers

April 2024

Brookhaven National Laboratory
Center for Functional Nanomaterials

Center for Integrated Nanotechnologies
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Center for Nanoscale Materials

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

REPORT OF THE BASIC ENERGY SCIENCES ADVISORY COMMITTEE
U.S. Department of Energy/Office of Science/April 2024

Prepared by the BESAC Nanoscience Research Centers Subcommittee

Report Number
PNNL-#####

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Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

Dr. Cynthia Friend
The Kavli Foundation
5715 Mesmer Avenue
Los Angeles, California 90230

Dear Dr. Friend:

Thank you for your continuing service as Chair of the Basic Energy Sciences Advisory Committee (BESAC). I appreciate the International Benchmarking report, which is inspiring similar assessments by other advisory committees in the Office of Science. Following on that report, I would like BESAC to take on a new charge.

The report found that the United States is falling behind other nations in critical aspects of the research enterprise, including key research areas, facilities and instrumentation, and the attraction and retention of talented people. It broadly recommended investments in research infrastructure, including experimental and computational facilities, career paths, and research and development integration from basic research to technological implementation. Going forward, it would be valuable to receive more specific advice on Basic Energy Science (BES) investment strategies. This charge concerns the area of facilities and instrumentation.

The first of the Nanoscale Science Research Centers (NSRCs) opened its doors for user research nearly 20 years ago. Today, the five NSRCs serve over 3,500 users annually, spanning a broad range of research topics and bridging synthesis/fabrication, characterization, and theory/modeling/computational/data science. Since their conception as user facilities, nanoscience has evolved from a new methodology addressing science and technology challenges to an established foundational capability for science and commercial technologies. Over this period, the capabilities at the NSRCs have expanded to include the electron microscopy user facilities as well as quantum information science.

At this juncture, I would like BESAC to examine the impact of the NSRCs to date and provide strategies for selecting high-impact, future directions for these facilities. Some questions that BESAC could consider in this study include:

- What has been the impact of the NSRCs? Consider scientific productivity, instrumentation advances, user community, contributions to national priorities, including energy technologies, and other metrics. What aspects of these facilities are “world-leading”?

- How are the collective NSRCs synergistic? What are the unique scientific roles?
- The initial vision for the NSRCs included synergies with the other user facilities at each of the laboratories. Has this vision been realized? What future directions are most promising?
- What are the best practices and opportunities for enhancement in the NSRC outreach activities to ensure a diverse user community?
- How should the NSRCs evolve to better serve the nation and user research?

It would be advantageous if BESAC approved the review report by the Spring or Summer meeting of 2024. I want to thank you and BESAC for undertaking this important function for the Office of Science.

Sincerely,

Asmeret Asefaw Berhe
Director
Office of Science

cc: H. Kung, SC-3
L. Horton, SC-32
K. Hochberger, SC-32

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Executive Summary

The five Nanoscience Research Centers (NSRCs) began operations during the period from 2006–2008, each associated with major Department of Energy (DOE) national laboratories. They aimed to bring state-of-the-art nanoscience instrumentation and expertise to a national user community, each with strong connections to a large user facility at its host laboratory. After two decades of operation, it is appropriate to assess the overall impact and consider the future for these facilities that serve a growing user community, now at over 4,000 unique users per year. This report, from a subcommittee chartered by the Basic Energy Sciences Advisory Committee, affirms that the NSRCs have made major positive impacts on materials and nanoscience research in the United States and beyond.

A review of these five facilities as a whole was also motivated by a recent BESAC study of international competitiveness, which singled out the importance of instrumentation development (also known as scientific infrastructure) and an instrument-savvy workforce. Freeman Dyson said: "New directions in science are launched by new tools much more often than by new concepts. The effect of a concept-driven revolution is to explain old things in new ways. The effect of a tool-driven revolution is to discover new things that have to be explained." We found that the NSRCs have played a signature role in advancing science and supporting innovations in instrumentation and techniques for nanoscience research. In addition, the NSRCs are a distinctive source of trained scientists and engineers. We echo the recent report from the National Nanotechnology Initiative[1] that conveys the ubiquitous nature of nanoscience in contemporary science and engineering, and that the tools of the NSRCs are critical for advances in most of today's science and technology grand challenge areas including energy, microelectronics, biotechnology, quantum information science, advanced manufacturing, high-performance computing, artificial intelligence, and autonomous systems.

The NSRCs complement investments from other agencies, such as the National Science Foundation (NSF), to build on DOE Office of Science expertise in user facilities for the service of a broad science and user community. Not only do they operate as proposal-based facilities, where users can access state-of-the-art instrumentation and computational capabilities at no cost (provided they publish their research in the scientific literature), but they also house experts who are dedicated to user support, perform world-leading science, and provide next-generation instrument development, largely free from the distractions of an academic environment.

This report not only documents the impressive impact of the NSRCs, using recognized metrics and a set of specific examples, it also charts a pathway to accelerate impact of the centers in the coming years, rising to the challenge of addressing emerging priorities and critical needs for U.S. competitiveness.

At the highest level, we recommend that the nation **sustain and strengthen** the collection of NSRCs that has become a key element of U.S. competitiveness in research on high-priority scientific problems and in instrumentation development. While the path forward includes an increased inventory of world-leading instruments and experts to support a growing user community, a major recommendation is for the **NSRCs to work cooperatively and synergistically** in addressing national grand challenges, with strategies developed in concert with BES and the user community. Early efforts to synergize so far have been very successful and should be greatly amplified.

The scientific brain trust of our nation is critical to international competitiveness. Since the NSRCs are a crucial source of scientists and engineers with both forefront research expertise and instrumentation skills, we recommend **expansion of** early career **training programs across the NSRCs**, as well as a **broadening of their user communities**, to address the human capital needs of the nation. The synergy with DOE and large facilities such as X-ray and neutron sources is very strong, and we recommend targeted investments to **leverage the ongoing upgrades** of these facilities.

KEY FINDINGS AND RECOMMENDATIONS

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

The success of the NSRCs lies in their exceptional combination of instrumentation and in-house expertise made available to many thousands of users. They also train many instrumentation-aware scientists and engineers, fulfilling a deficit in U.S. competitiveness.[2]

While the NSRCs 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.

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 centers should take advantage of opportunities to work collectively and provide international leadership in priority scientific areas. In doing so, the NSRCs should ensure ample engagement with the broader community of scientists. Essential to this leadership is a prioritization of 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.

The NSRCs have achieved remarkable success since their inception, enabled by individual focus from each center to build the user community, hire and develop staff, and acquire and develop instrumentation. But today it is clear that their impact could be greatly boosted by a new level of cooperation and planning. The broad expertise of the NSRCs, in its totality, represents a leading force that can help the United States regain international leadership in instrumentation-enabled science.

A major move toward synergy would be the development of a single portal for proposals for all NSRCs and a challenge to the user community to generate proposals that take advantage of multiple facilities and develop mechanisms that promote multifacility utilization. A challenge is to simplify the process for users through a single portal for user proposals. NSRCs should continue efforts to use advances in remote access capabilities that were established during the COVID-19 pandemic, which could also increase engagement of non-R1 Minority Serving Institutions (MSIs) and Emerging Research Institutions (ERIs) in the user community.

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 programs supporting early career scientists, post-doctorates, and staff 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 U.S. 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.

The decision to co-locate the NSRCs with other DOE capabilities was a prescient strategy and 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.

Ongoing emphasis of the NSRCs on broad outreach is critical for increasing impact and the elevation of science and technology from historically underrepresented 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.

The NSRCs have experienced good but limited success in industrial interactions that represent a growing opportunity in areas such as microelectronics and quantum information sciences. 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, and the technologies developed have had impact beyond the NSRC user community. In parallel, they have been very effective in connecting with small companies associated with technology spinoffs, contributing 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. Doing so would not only advance the technical objectives of the industrial users for further economic growth, but also expose NSRC scientists to frontier research questions that are of particular importance to industry in their efforts to advance technology. More extensive interactions with industry beyond the user program, e.g., through affiliates, focused short courses, and invited seminars, would be valuable.

SECTION 1

Introduction

The 21st Century Nanotechnology Research and Development Act[3] signed by President George W. Bush in 2003 led to the implementation of major investments at several agencies in nanoscience and technology reflecting the growing importance of “nano” in science and engineering. The far-seeing aim of the initiative was to implement a *shared vision of a future in which the ability to understand and control matter at the nanoscale leads to ongoing revolutions in technology and industry that benefit society*.

The most recent strategic plan of the National Nanotechnology Initiative (2021) emphasized the major impact of nanotechnology on society; nanoscience has become ubiquitous in almost all areas of science and engineering.[4] We have always known that materials are controlled by their organization on the nanoscale, but only in recent years have we learned to understand, control, and optimize nanostructures to the benefit of technology and society.

The Department of Energy’s (DOE’s) signature investment in infrastructure for nanoscience was the creation of five scientific user facilities comprising the Nanoscale Science Research Centers (NSRCs): the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory; the Center for Integrated Nanotechnologies (CINT) at Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL); the Molecular Foundry (MF) at Lawrence Berkeley National Laboratory; the Center for Nanoscale Materials (CNM) at Argonne National Laboratory; and the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (listed in order of their founding). As demonstrated in Figure 1, which shows some of the distinctive and complementary aspects of the NSRCs, each center stewards a small set of very specialized instruments, together with a broader set of characterization, synthesis, and processing tools where there is often appropriate overlap with other centers. Often truly unique instruments leverage the large user facilities at each laboratory, such as light sources, neutron sources, and micro/nanoelectronics fabrication facilities. Figure 1 is not comprehensive (such information can be found in the rest of the report and in the web pages of each facility) but demonstrates one or two distinctive capabilities at each facility while also listing some of the capabilities that are common to all.

The subcommittee on the NSRCs was established by the Basic Energy Sciences (BES) Advisory Committee, in response to a charge from the Director of DOE’s Office of Science to assess the NSRC’s impacts and future directions. The subcommittee includes leading domestic and international experts covering broad areas of nanoscience, and representing universities, national laboratories, and industry. The subcommittee held several meetings and one in-depth workshop with representatives from the NSRCs, including their directors, and BES. Extensive data were requested and provided by the centers and BES staff. All of this supplied the information needed for an assessment of the impact of the entire ecosystem, specifically to answer the five questions in the charge letter (included as a preface to this report). Each question is addressed in the following chapters, which also presents the evidence to support the consensus recommendations. Note that the subcommittee avoided reviewing the centers as individual entities; this is done periodically and in great depth via peer review organized by BES. Instead, this subcommittee looked holistically at the collection of centers, assessing not only their impacts but also the factors that have led to these impacts, and evaluated a path forward to maximally leverage future investments in the centers. Section 2 contains an evaluation of the impact of the centers up until the present, including metrics and selected highlights of the output.

SECTION 2

Impact of the Nanoscience Research Centers

There are five NSRCs located at six national laboratories, mostly co-located with other BES-supported user facilities. The research focus and capability investments for each NSRC are well aligned with other BES user facility instrumentation and capabilities, creating synergy for advancing new scientific opportunities. Some of the signature elements available within each facility are highlighted in Figure 1 and Figure 2 below. With the NSRC vision of providing state-of-the-art nanofabrication and characterization facilities to advance science by serving the scientific community, the ability to have multiple capabilities and expertise housed in a single facility provides an advantage relative to a more distributed model in streamlining research for the users. Several examples of unique developments advanced through this embedded model will be presented later in this report.

While the centers have distinctive and critical activities, there is also overlap in some of the research areas and capabilities. Because of the embedded expertise model used by the centers, each center needs to have broad capabilities and thus some overlap, and duplication is to be expected and is desirable. The breadth also benefits users who find it convenient to access facilities nearer to their home laboratory. At times, the NSRCs have used this overlapping expertise to deliver added impact, as in the case of microscopy discussed in Section 3 (Highlight 6). While all the NSRCs have electron microscopy facilities, each has unique expertise in specific areas of microscopy that sets them apart from each other. The NSRCs have taken similar approaches in other areas including scanning tunneling microscopy, scanning probe microscopies, and synthesis capabilities. Through the cross-center collaboration model currently being developed, deeper understanding of the common capabilities across the NSRCs will be established, providing enhanced facility access overall. For example, when a particular NSRC facility may not be able to host additional research work, such knowledge of duplicative capabilities could enable that research work to be pursued at other facilities. While this type of model is not yet fully in place, it is an exciting opportunity: the promise for increased NSRC scientific impact will more than justify the efforts needed to provide an improved system for enabling cross-NSRC collaboration.

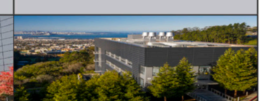
NSRC	CFN	CINT	CNM	CNMS	Foundry
					
Specialized Capabilities	In situ and operando X-ray and electron microscopy and spectroscopy	Microelectronics and quantum device fabrication	Hard X-ray nanoprobe beamline	Automated flow reactor for polymer synthesis and site-specific deuteration	Terahertz scanning 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				

Figure 1. Specialized capabilities and strategic directions of the NSRCs, with a list of overlapping capabilities.

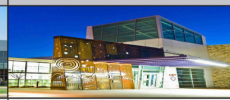
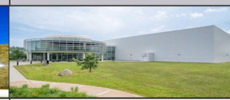
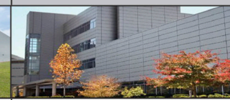
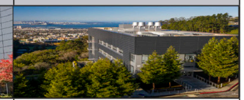
CFN	CINT	CNM	CNMS	Foundry
				
• Quantum Material Press (QPress) for automated synthesis of layered heterostructure materials • FEI Titan 80-300 E-TEM instrument has a differentially pumped environmental cell for in situ observation and gas-reaction experiments • XPEEM/LEEM facility at ESM 21-1D-2 beamline at NSLS-II—full-field imaging, uXPS, uXAS, uARPES • Soft Matter Interfaces (SMI) beamline at NSLS-II to study structure, energetics, and assembly of soft materials • Ambient Pressure XPS and UPS with in vacuo IRRAS for surface chemical analysis	• Metamaterials and nanophotonics • Microelectronics and quantum device nanofabrication • Multiple dilution refrigerators for LT transport and quantum materials • Raith nano-implantation system quantum defects • Oxford Instruments deep reactive etch tools for high aspect ratio etching of semiconductors • ntlvax thin film dual ion beam spluttering systems • Nanonics Imaging multi-probe system for nanometric positioning paired with collocated physical, chemical, and optical characterization	• CNM/APS Hard X-ray Nanoprobe Beamline for 3D Bragg ptychography and nano-XRF imaging • Ultrafast electron microscope (UEM) and ultrafast pulsed CL/PL Cs-corrected STEM • Polybot – suite of autonomous synthesis capabilities, including home-grown AI software for accelerated discovery • Quantum labs – optically coupled ultralow temperature dil fridge and ADR with high-field broadband ODMR • Light-coupled 4K STM to excite and analyze surface defects	• Niron HERMES cryogenic monochromated aberration-corrected STEM (MAC-STEM) + Nion IRIS ultra-high energy resolution EELS • Cameca/Ametek local electrode atom probe (LEAP) 4000X HR and cryo-plasma FIB needle prep • Unisoku spin-polarized 4-probe STM and Scienta Omicron vector-field milli-Kelvin (mK) STM • SPECS Joule-Thomson UHV SPM for tunneling spectroscopy • Polymer synthesis: Automated Flow Reactor System (AutoFlowS) and capabilities for site-specific chemical deuteration	• HERMAN – custom robot for synthesis of inorganic, organic, and hybrid nanomaterials; WANDA – custom automated robot for synthesis of colloidal inorganic nanomaterials • QIS gas-phase multi-chamber UHV cluster tool for deposition of metals, oxides, and nitrides • THz STM/AFM • FEI TEAM I – correction of geometric and chromatic aberration in TEM and STEM modes • FEI TEAM 0.5 – aberration-corrected STEM with LBNL-developed 87 kHz 4D camera

Figure 2. Each NSRC supports its strategic foci (Figure 1) with distinctive signature instrumentation.

Overall growth in the NSRCs has progressed rapidly since their implementation, a testimony of the value that these centers provide to the scientific community. Since 2007, there has been a nearly linear increase in the number of users on a yearly basis (Figure 3), with the user base more than doubling in the 10 years between 2009 and 2019. Although the user base took a dip during 2020–2021 associated with the pandemic, in the first year back with more normal operations, the user base largely resumed the healthy growth trajectory. New modes of working were established during the pandemic and, as a result, the NSRCs are more flexible and have facilitated nearly a third of the users to be remote enabling further research impact: to date users from a combined 49 states and more than 50 countries have benefitted from the NSRC capabilities.

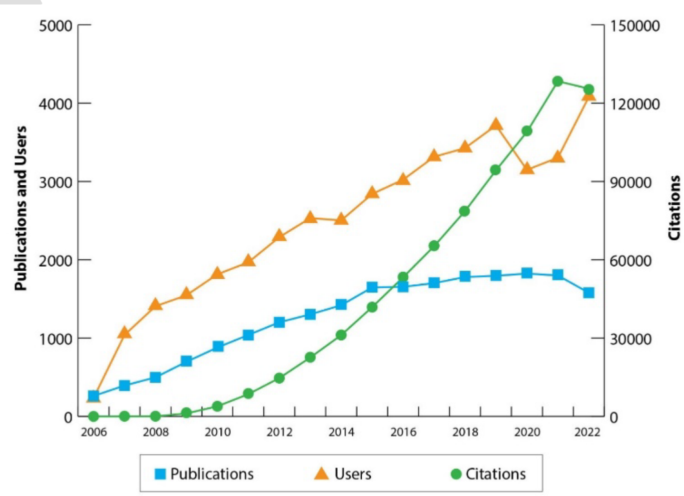


Figure 3. Annual number of refereed publications, unique users, and citations for the NSRCs. Note the recent pandemic impact, first on users, then on publications and citations.

PUBLICATIONS AND PATENTS

Research conducted within the NSRCs has been translated into numerous refereed publications with strong growth through 2016, although the publication rate appears to have slowed in recent years despite the strong growth in the user base (Figure 3). The impact of the pandemic is in 2020–21 for all metrics. Additional plateauing in publications beginning around the 2015–2016 timeframe appears to correlate with funding and staffing challenges facing the NSRCs; an added challenge is the increasing complexity of user experiments as the facilities have matured. Most recent data show a good record of publication, with 1,017 total publications for all the NSRCs in 2023 to date, and 54% of those publications in journals with an impact factor >7, including 94 publications in the *Nature* portfolio and 14 publications in the *Science* family.

While publications are one measure of NSRC productivity, citations are indicative of the continuing impact of the science. Because there is a lag between publication and citation, it is difficult to compare these two numbers directly. The citation data collected show a continuous increase in citation frequency (Figure 3). The recent drop off is likely related to the pandemic, and further data will be needed to better understand the more recent trend. The strong citation record clearly points to significant impact from the science being enabled through the NSRCs.

Intellectual property is another measure of impact. With nearly 350 patents created from the NSRC science (Figure 5), there is strong evidence of a translation of the science to technology. While there is more scatter in the data, a similar plateauing is found for intellectual property

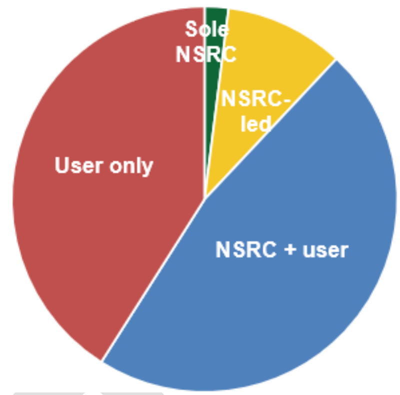


Figure 4. Authorship of publications shows a high degree of collaboration between users and NSRC researchers (data for 2022).

(IP) generation as was seen for publication output (Figure 5; Figure 3). Patents are not necessarily a measure of value in and of themselves, and further valuation metrics are seen both through awards and licensing or commercialization examples. The NSRCs also have an impressive total of 46 R&D 100 awards between them.

Several of these technologies have been moved into startups and/or licensed. Some notable examples include the technology transfer of magnetite nanoparticles into clinical trials with Imagion Biosystems, and the BADx technology, which was licensed to Aquila for use in diagnostic equipment for detecting anthrax. It is unclear how/whether the availability of the NSRC IP is publicized to potential larger industrial organizations. Broader utilization

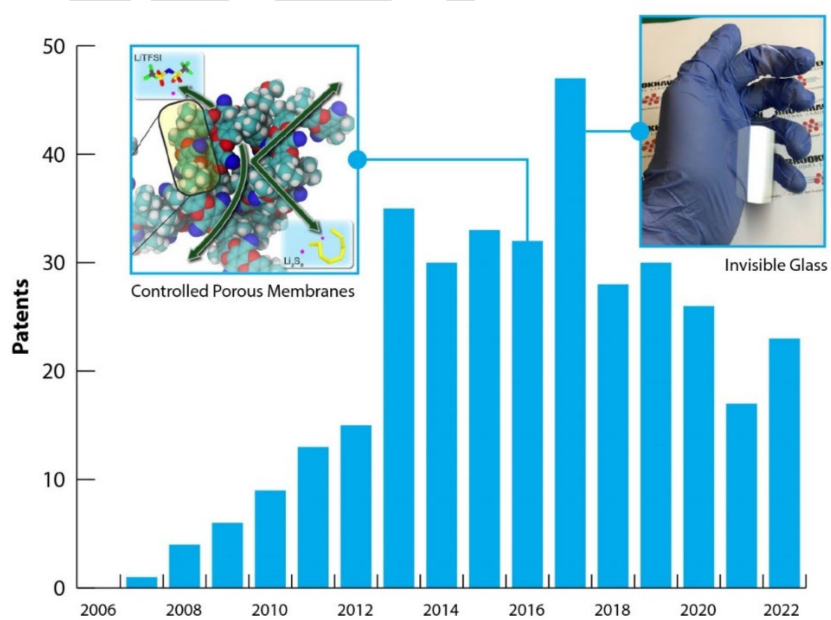


Figure 5. Annual patent production by the NSRCs.

would further enhance the value of the technology and bring maximum impact to the NSRCs. Many of the national laboratories offer competitive fellowships for small business entrepreneurs that provide access to resources at the lab; this includes access to the respective lab's NSRCs (through the standard proposal submittal process). These small business "incubator" programs are listed below:

1. Oak Ridge National Laboratory – *Innovation Crossroads*
2. Argonne National Laboratory – *Chain Reaction Innovations*
3. Lawrence Berkeley National Laboratory – *Cyclotron Road Innovators*
4. Sandia National Laboratories – *Center for Collaboration & Commercialization*

Figure 6 highlights several small businesses entrepreneurs participating in Argonne's *Chain Reaction Innovations* program, which are typical. These companies cannot afford renting lab space, purchasing expensive equipment, and training new people. The NSRCs can provide these assets and capabilities to help companies get off the ground successfully for free. In some cases, the principal investigator (PI) was a user at the CNM (who later formed a startup and continued to use the CNM).

LEADERSHIP OF NSRC STAFF

Up to this point, scientific and technological advancements have been assessed as a basis for determining impacts of the NSRCs, but these are only partial measurements of their influence. The researchers at the NSRCs are leaders in their fields, and each NSRC has staff members who started at the center as either a student, user, or postdoc and have established independent, successful careers at the NSRC or elsewhere. One stellar example is Nobel Prize winner Carolyn Bertozzi, who was formerly a director of the Molecular Foundry. Other examples of the impact of training by the NSRCs are demonstrated in Highlight 1.

The demographics for the NSRC staff reveal a healthy distribution of experience with more professionals having under 10 years of NSRC experience than over 10 years. Retention data suggest there is about a 10% loss rate for the NSRCs overall. It is unclear what career stage is being most impacted by staff departures, which is something that should be monitored to ensure a healthy pipeline is maintained. Postdocs have also been successfully transitioned into the NSRC staff, helping to continue growing the talent pool.

Overall, the NSRC staff are internationally recognized as leaders in their fields. For example, there are 31 NSRC researchers serving as Society Fellows across a range of

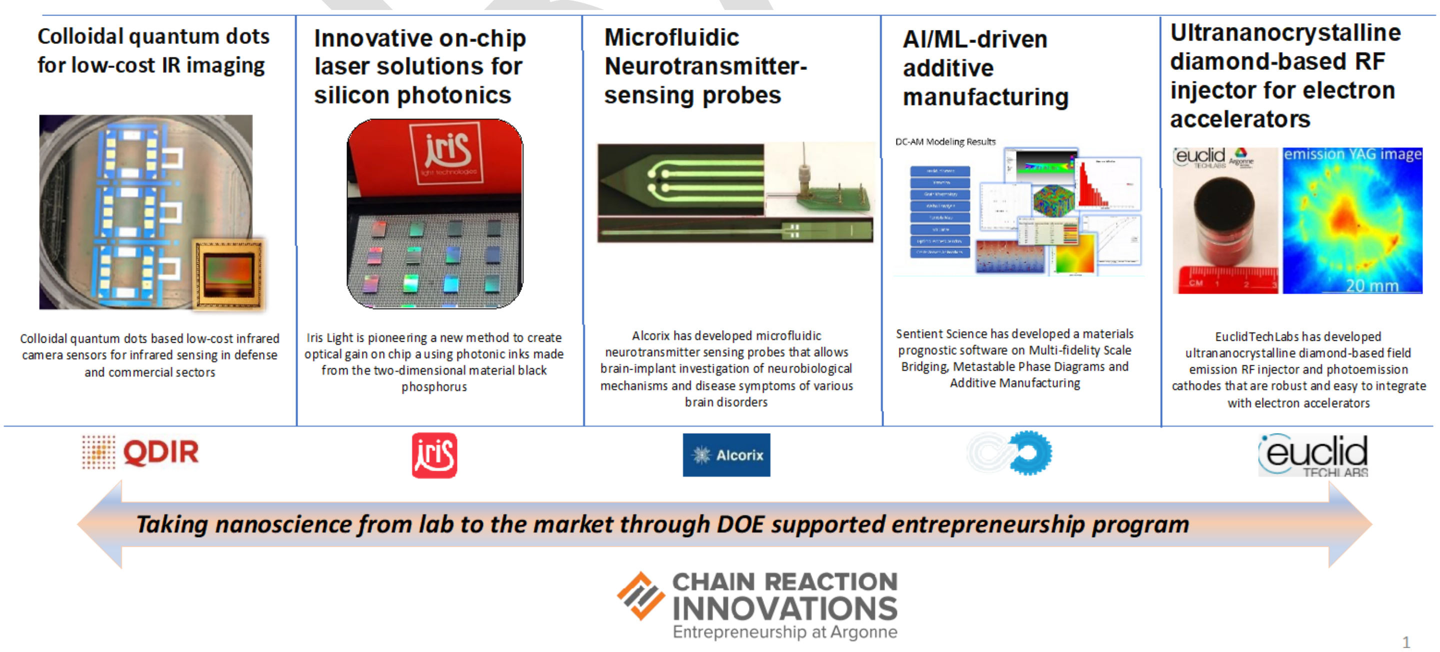


Figure 6. Argonne's Chain Reaction Innovations program is one example of how NSRCs have been translated to the marketplace.

fields, with nearly 40% of those fellows in the American Physical Society. Considering the broad remit, society participation may be an area to review to ensure that the NSRCs are having the broadest scientific leadership possible and are not focused too much in one area. The NSRCs are also well represented in research society leadership roles. A listing of the current society leaders is presented below.

Important Society Leadership Roles for Current NSRC Staff:

- *Andy Minor* – President, Microscopy Society of America (MSA)
- *Peter Ercius* – Director, MSA Physical Sciences
- *Brad Boyce* – President, The Minerals, Metals, and Metallurgical Society (TMS)
- *Ilke Arslan* – Materials Research Society, Board of Directors
- *Brad Lokitz* – Society for Science at User Research Facilities (SSURF), Board of Directors
- *Jordan Hachtel* – Microanalysis Society (MAS), Board of Directors

The NSRC staff has also been recognized with some notable awards and honors. A short list is presented below.

Notable Awards and Honors for Current NSRC Staff:

- MSA Burton Medal – *Miaofang Chi, Colin Ophus, Andy Minor*
- Presidential Early Career Award for Scientists and Engineers – *Ilke Arslan, Elena Shevchenko, David Cullen, Jim Ciston*
- MSA Crewe Award – *Jordan Hachtel*
- MAS Heinrich Award – Miaofang Chi, Jordan Hachtel
- National Academy of Science & Technology of the Philippines – *Rigoberto Advincula*
- TMS Cyril Stanley Smith Award – *Kristin Persson*
- National Academy of Engineering – *Gary Grest*

HIGHLIGHT 1: TRAINING AND ENABLING LEADERS


Katherine Jungjohann


Jeffrey Neaton


Armando Rúa


Rama Vasudevan


Jana Zaumseil

A core strength of the NSRCs rests with their emphasis on training emerging scientific leaders in highly specialized techniques, as well as in interdisciplinary and collaborative scientific thinking. By bringing together exceptionally talented researchers and enabling them to focus on pressing challenges, the NSRCs represent a powerful training ground for scientists.

Katherine Jungjohann joined the Center for Functional Nanomaterials as a postdoctoral researcher in 2012, where she used liquid cell electron microscopy to understand the nucleation and growth of nanostructures. Upon finishing her postdoctoral work, she moved to the Center for Integrated Nanotechnologies where she led the development of microelectromechanical system device fabrication to advance in situ scanning/transmission electron microscopy capabilities. In 2021, Katherine moved to the National Renewable Energy

Laboratory (NREL) to lead a group that provides advanced analytical microscopy and imaging characterization to NREL staff and collaborators.

Jeffrey Neaton started at the Molecular Foundry in 2003 as a postdoctoral researcher and transitioned to a staff scientist role in 2005. A decade after joining the Molecular Foundry he became its director, serving from 2013–2019. Jeff's research develops and uses theoretical and computational approaches to understand and design materials. Multi-disciplinary collaborations with experimentalists feature prominently in his work, an approach honed over many interactions with users over the years. A Fellow of the American Physical Society, Jeff is currently the Associate Laboratory Director for Energy Sciences at Berkeley Lab and a professor of physics at the University of California, Berkeley.

Armando Rúa is an associate professor of physics at the University of Puerto Rico-Mayagüez and a user at the Center for Functional Nanomaterials. His research generally focuses on using fundamental science insights to develop functional thin film materials for applications such as electronics and sensors. Armando was named a 2023 Experimental Physics Investigator by the Gordon and Betty Moore Foundation, receiving funding for work to understand how switching occurs when materials transition from metallic to insulating states. These materials could be used for computing hardware inspired by the human nervous system.

Rama Vasudevan joined the Center for Nanophase Materials Sciences in 2013 as a postdoctoral researcher working with scanning probe microscopy. Rama has remained at the Center for Nanophase Materials Sciences throughout his career, assuming a group leader role in 2022. His expertise centers on developing autonomous synthesis and characterization tools. Autonomous systems require intelligent machine learning that engages with domain science expertise, enabling rapid decision making. Rama was part of a team whose software suite for autonomous experimentation received a 2023 R&D 100 award.

Jana Zaumseil worked at the Center for Nanoscale Materials as a postdoctoral fellow from 2007–2009. During her tenure there, she studied the transport properties of carbon nanotubes. Her work revealed properties about the bandgap and defects in semiconducting carbon nanotubes. After her postdoctoral work was completed, Jana has held multiple professorships in Germany and is currently the chair for applied physical chemistry at Heidelberg University. Her research still centers on semiconducting carbon nanotubes, including how charge moves through these materials, understanding how defects interact with light, and how to apply these materials in nanostructured devices.

Such external recognition also points to the impact and influence the NSRCs have in the scientific and technical communities. While the NSRCs are certainly leading in scientific advancements, it is harder to judge whether the capabilities of the NSRCs are world leading. The one benchmark assessment by *U.S. News and World Report* is limited to universities.[5] In this listing, eight of the ten top universities were in China, with the two domestic universities supported through the NSF National Nanotechnology Coordinated Infrastructure (NNCI). Given the broad remit of the NSRCs to embed both nanofabrication and characterization capabilities, it is difficult to maintain leading edge capabilities in all areas. The microscopy initiatives currently under discussion for the NSRCs will drive future world-leading microscopy capabilities. The NNCI has a narrower lens of focus to maintain a prioritization of resources on nanofabrication to maintain a competitive edge.

The NNCI has a complementary model to the NSRCs. An attempt to compare the two models is given in Table 1. Two NSRC directors serve on the external advisory boards of leading NNCI nodes (Karren More serves on the board of the Southeastern Nanotechnology Infrastructure Corridor; Chuck Black is chair of the science advisory board for the Cornell Nanoscale Facility), and thus have familiarity with both models and provided the background information included in the table.

The two systems form a strong backbone for the United States in nanoscience leadership, with NNCI providing industrial users access to capabilities they may not have in-house and the NSRCs providing a strong steer toward the

Table 1. Comparison of the NNCI and NSRCs

	NNCI	NSRCs
Operating Model	16 facility nodes located on university campuses across the United States.	Five NSRCs located at six US National Laboratories. Leverage other on-site user facilities (e.g., light and neutron sources).
Mission	Provides and supports scientific facilities for users, and primarily supports users through training and professional experience.	Provides and supports facilities for users. Staff are also engaged in their own leading research. NSRC scientists are involved in developing and supporting unique, leading-edge instrumentation.
Facilities	Focuses on micro/nano fabrication conducted in cleanroom environments and extensive characterization instrumentation, including electron microscopy.	Offer a broad range of capabilities, including nanofabrication and characterization using electron, X-ray, and laser-based probes, scanned-probe and surface science instrumentation, and theory and computation facilities for understanding nanomaterials.
Facility Access	Users pay an hourly fee to access instruments across all NNCI nodes. No peer-review proposal process needed to access facilities.	User access to NSRCs is granted through external peer review of submitted proposals, after which facility use free for open research. Proprietary research access is available for a fee, following a successful review process
Funding	NSF funds a portion of the facility operating costs (some portion of maintenance and staff), requiring supplementary funding from other sources.	The DOE fully funds the operating costs of NSRC facilities.

future of nanoscience such that both approaches serve the short-, medium-, and long-term needs in this scientific space. One disadvantage of the NSRC approach is that there is less industrial engagement, which could mean that important scientific challenges are not being recognized by the research community, limiting them from the scope of consideration for investigation. If the peer review of research proposals does not have appreciation of industrial needs and interests, they may not be able to fully evaluate the proposal's relevance. Simultaneously, the NNCI approach could lead to very short-term/tactical advances and miss important areas where they could be contributing to scientific advancement. This is balanced partly by having these centers embedded into world-leading academic institutions, but it is still recognized as a risk for the approach. Clearly the United States benefits from the complementarity of the agency approaches that is often absent in other countries.

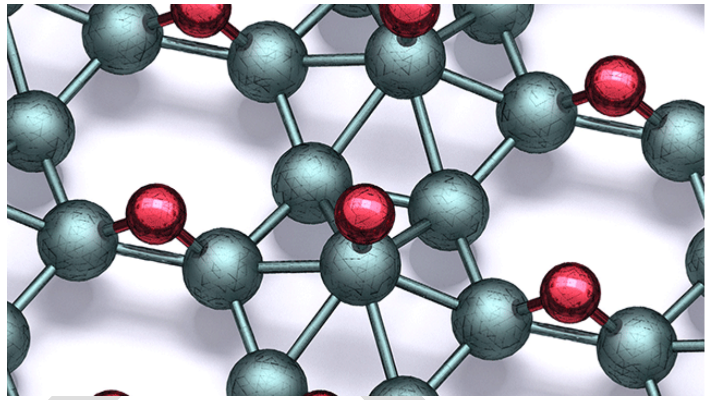
One of the major areas of concern is that the increasing number of users for the NSRCs may be slowing progress of research advancement, as each NSRC will have some maximum carrying capacity past which there are challenges to adding additional users. The publication and IP records described previously provide potential evidence that this may already be surfacing, and this limit should be evaluated in terms of adequate staffing and instrumentation.

CONCLUSIONS

The NSRCs provide users not just with state-of-the-art equipment, but more important, access to leading researchers who both work with users and maintain NSRC-based research programs to develop the expertise and capabilities for future users. This model is unique and helps the NSRCs achieve significant impact, through the user program and user publications as well as high impact scientific publications led by NSRC staff. The NSRCs have also created IP that led to commercialization and translation of scientific discoveries made within the NSRCs. Since travel and housing costs can impede participation by academic users, it is important to preserve the current model where there is some duplication of core capabilities, while each NSRC develops distinctive expertise that leads the field. The centers have a coordinated approach toward adding new capabilities, as evident in their strategic plan and recapitalization goals. In terms of industry engagement, there has been good success with smaller startup companies who can take advantage of the nonproprietary usage model. Larger U.S. corporations have limited involvement with the NSRCs unless there is a champion in-house. The NSRCs could enhance their dialog with U.S. industry through other means beside user proposals, such as participation in advisory boards or visits to industry by NSRC scientists describing their capabilities and research outputs.

HIGHLIGHT 2: BORON IN TWO DIMENSIONS

Boron is a highly versatile element, with the ability to form multiple covalent bonds and molecular networks. These similarities to carbon, including in the behavior of small cluster structures, led researchers to predict that a boron analog of graphene should exist. In 2015, researchers from Argonne National Laboratory and Northwestern University created borophene—a 2D sheet of boron—for the first time at the Center for Nanoscale Materials (CNM)[6].



A representation of borophane, a two-dimensional sheet of boron (gray spheres) bonded to hydrogen (red spheres) for increased stability. *Image by Mark Hersam, Northwestern University.*

The atomically thin material formed in crystalline sheets on silver surfaces in an ultrahigh vacuum, its structure resembling fused clusters of boron. Rather than a fully flat surface, there is substantial out-of-plane buckling that produces boron islands. Borophene behaves differently from bulk boron, with characteristics of an anisotropic 2D metal.

Despite its exciting properties, borophene is highly unstable outside of a vacuum. It rapidly oxidizes in air and loses its conductivity, making it impractical for most applications. Recent advances led to the synthesis of hydrogen-functionalized borophene known as borophane. In an ultrahigh vacuum, adding atomic hydrogen to borophene leads to borophane. Borophane has a range of potential structures, but with help from a computer-vision-based tool developed by CNM scientists called Ingrained, the team was able to determine the structure of borophane from scanning tunneling microscopy images and quantum mechanical simulations. They found that the most common structure has a mixture of single boron-hydrogen bonds and three-center–two-electron boron-hydrogen-boron bonds.

Like borophene, borophane has clear metallic characteristics. Unlike borophene, borophane is stable in ambient conditions and can be easily converted back to pure borophene by heating. This dramatically widens the range of potential uses for 2D boron structures. Source: *Science* 350, 1513 (2015); *Science* 371, 1143 (2021)

HIGHLIGHT 3: USING MACHINE LEARNING TO DISCOVER NEW SUPERCAPACITORS

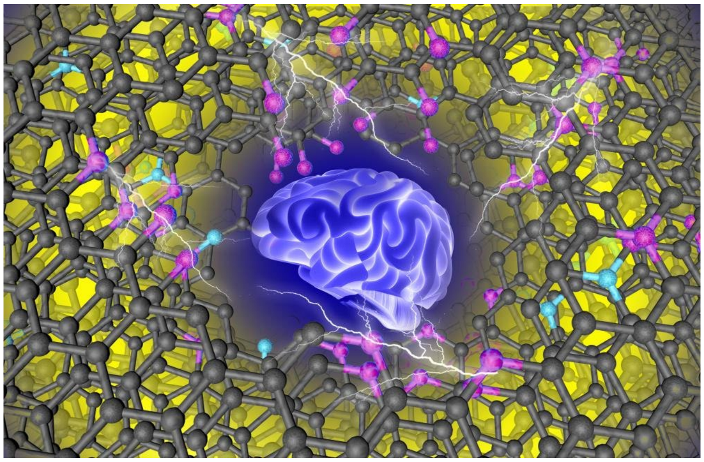


Image by Tao Wang, Oak Ridge National Laboratory.

Water-based supercapacitors are essential for applications that require large amounts of power to be stored for an extended period of time, such as regenerative brakes and power electronics. Porous, carbon-based materials are currently the primary focus of much research into these supercapacitors. However, finding new and improved materials traditionally relies on labor-intensive synthesis and characterization methods.

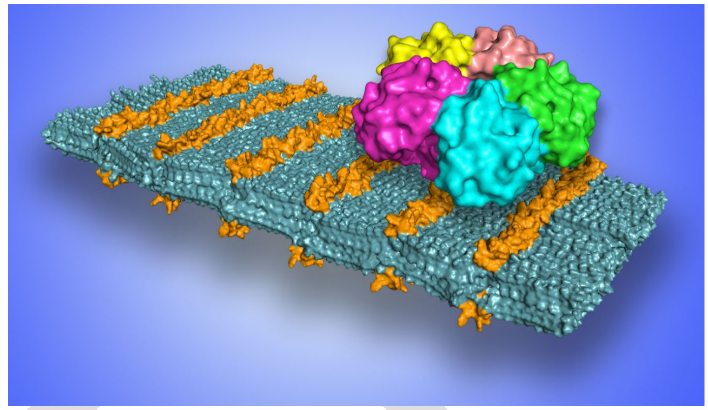
By using machine learning (ML) guidance, Oak Ridge National Laboratory researchers worked with staff at the Center for Nanophase Materials Sciences (CNMS) to design a carbon-based supercapacitor capable of storing four times more energy than current commercial technology. The team built an artificial neural network model trained to develop the best possible electrode for holding a charge. The model predicted that doping nitrogen and oxygen into the carbon structure would lead to the highest capacitance.

By tuning the size of the pores and oxygen content in the carbon-based electrode, the research team was able to produce a capacitance near that predicted by the ML model. Further study found that the key to the high capacitance was a combination of multiple pore sizes, providing both a high surface area and channels that facilitate electrolyte movement through the material. Mapping the pores was challenging due to their disparate sizes, and resources at CNMS played an important role in understanding pore distributions and structure. This work is a powerful demonstration of how leveraging ML can accelerate materials discovery.

Wang, T., *et al. Nature Communications,* **14,** 4607 (2023). [DOI: 10.1038/s41467-023-40282-1]

HIGHLIGHT 4: TARGETING PATHOGENS WITH PEPTOIDS

Peptoids are a class of molecules that mimic proteins but feature enhanced stability and significant tunability. Researchers at the MF have extensive experience working with peptoids, generating over 150 publications and five spinoff companies since 2006 focused on these biomimetic materials.



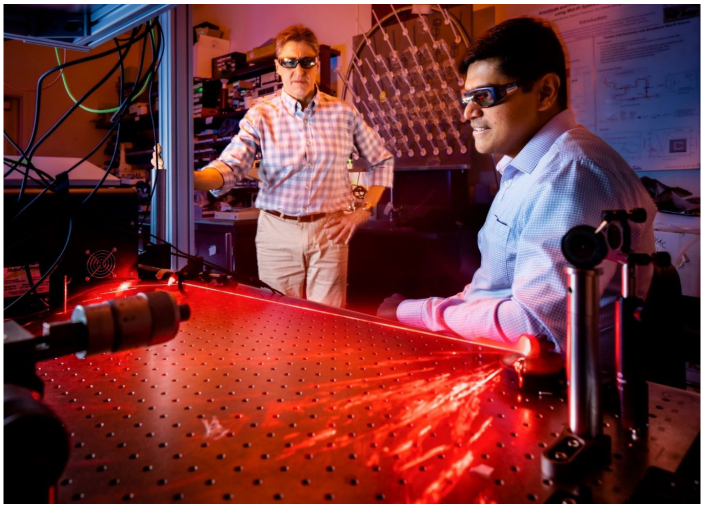
A molecular model of a peptoid nanosheet showing sugar-based loop structures (orange) that bind to the Shiga toxin (the five-color bound structure). *Image by Berkeley Lab.*

Using MF resources, researchers developed a process for creating ultrathin, self-assembling peptoid sheets with loop structures on both sides. These loops, which are made from simple sugar molecules, can selectively bind to several different proteins. By adding fluorescent probes to the peptoid and protein, researchers were able to confirm binding with a color change in the emission.[7]

The loop-embedded nanosheets are a versatile platform that mimics the exterior of cells, but with enhanced customizability. Selecting a different sugar loop or other structure to incorporate into the sheet can alter the protein that binds to the peptoid. This enables scientists to use the general framework for a wide range of potential applications, from environmental remediation to pathogen detection, as shown in the research through successful binding of a protein associated with the Shiga toxin that causes dysentery.

Source: *ACS Nano*, 2018, 12, 3, 2455–2465. [DOI: 10.1021/acsnano.7b08018]

HIGHLIGHT 5: SEMICONDUCTOR METASURFACES EMISSION



The hardware used for beam steering experiments at the Center for Integrated Nanotechnologies (CINT). *Image by Craig Fritz.*

Traditionally, applications that require light steered in specific directions have relied on lasers combined with bulky and complex electromechanical systems. Researchers from the Center for Integrated Nanotechnologies (CINT) used a semiconductor device that directs light from conventional and incoherent sources (such as LED bulbs, incandescent lamps, etc.) in precise directions.

The research team employed a metasurface—a semiconductor-based, artificially structured material—embedded with light-emitting quantum dots. Using a grating-like refractive index pattern programmed onto the metasurface, they were able to steer the light emitted from the quantum dots over a 70-degree field of view and at sub-picosecond time scales. This result demonstrated for the first time that incoherent light could be steered in a programmed direction.[8]

This work represents an exciting proof of principle for integrating an incoherent light source with a metasurface that can be programmed to steer light into specific directions. Ultimately, the researchers are aiming to develop a combined LED and semiconductor metasurface where steering will be achieved by simply applying a voltage to additional control electrodes. Developing an approach to dynamically control incoherent light sources, which include low-cost devices such as LEDs, could lead to a wide variety of new applications that range from holographic and augmented/virtual reality imaging, to communications, to ranging devices for autonomous vehicles.

Source: PP Iyer et al., Nature Photonics 17, 588-593 (2023). [DOI: 10.1038/s41566-023-01172-6]

SECTION 3

Collective Synergy among the Nanoscience Research Centers

DOE's NSRCs provide access to forefront scientific instrumentation and expert support for the national and international research community. Each center has core capabilities in nanofabrication, materials synthesis, characterization, and theory and computation. However, each facility has unique strategic scientific directions aligned with DOE priorities, host-lab interests, and strengths. These, in turn, led individual NSRCs to establish distinct capabilities for each center and extend beyond the core capabilities required for nanoscience research. This collection of world-leading experimental tools (Figure 1 and Figure 2) provides opportunities for the research community to access and exploit the highest caliber of instrumentation and methods to advance their own research efforts.

One way to describe how the NSRCs are collectively synergistic is with respect to the efforts in materials characterization with electron microscopy. Each of the NSRCs has substantial, forefront electron microscopy facilities; however, each NSRC has a unique area of scientific emphasis, which informs the choice of instrumentation and has led to the establishment of specific national Centers of Excellence. The MF's transmission electron achromatic microscope (TEAM) instruments and early adoption of direct electron detectors have resulted in atomically resolved, three-dimensional (3D) tomography capabilities and the development of 4D scanning transmission electron microscopy. The CNMS is a world leader in scanning transmission electron microscopy and high-resolution electron energy loss spectroscopy. The CNM has unique dynamic and ultrafast electron microscopy instrumentation. CINT has developed capabilities for studying ion-beam damage in materials and cryogenic electron microscopy (CryoEM) for energy storage materials. The CFN focuses on in situ and operando environmental microscopy approaches. This collection of capabilities represents a form of synergy between the centers in that efforts are not duplicative and provide a broad range of forefront capabilities to the research community. These efforts are further bolstered by other materials characterization capabilities such as scanned probe microscopies, synchrotron-based instrument partnerships, atom probe tomography, and more.

The NSRCs also coordinate activities in response to DOE requests, funding opportunities, and in response to areas of national scientific need. In one example, the NSRCs recently coordinated efforts to recapitalize. Here, the five centers prepared a joint proposal to DOE to secure the funding and organized a guiding framework for the instrument selection based on three strategic focus areas in nanoscience (Figure 7). Each Center made internal decisions on their priorities, aligned with their strategic scientific directions. These decisions were then

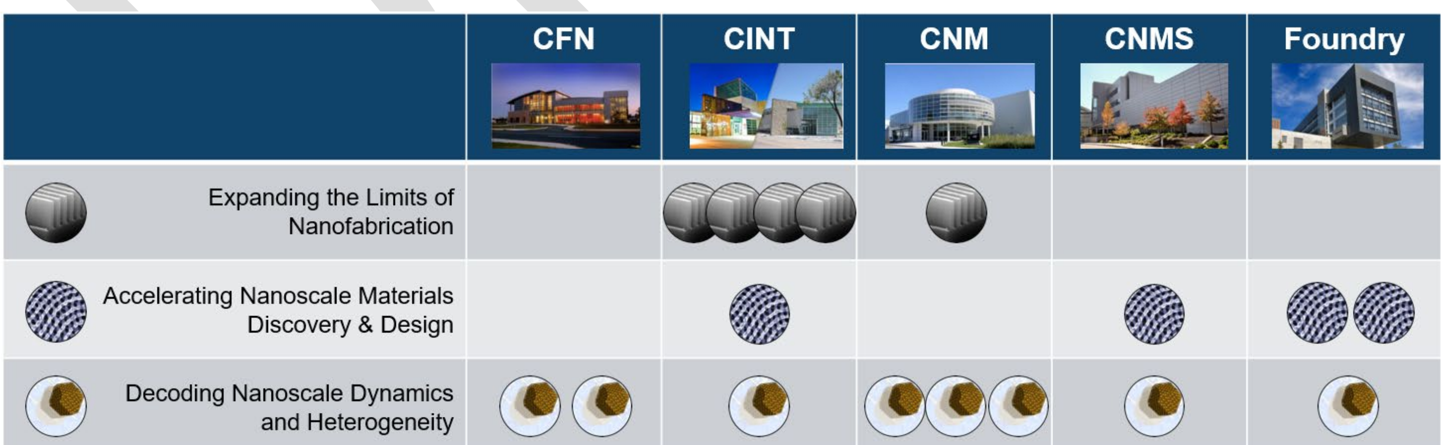


Figure 7. Recent recapitalization efforts at the NSRCs focused on three specific areas of nanoscience (left column). Instrument investments at each facility were made to align with these areas and enhance facilities' efforts to support their strategic foci.

amalgamated and distributed across the three strategic focus areas. This again led to the development of distinctive instrumentation being placed at each facility in a way that did not create duplication of capabilities.

In addition, the NSRCs work to develop synergies in their operations. Monthly meetings between the NSRC directors and user program managers help to articulate and incorporate best practices for operations, allowing more efficient and effective center management. Areas of focus include reporting, outreach, yearly user meetings, data collection, proposal review processes, and facilitating remote usage and self-driving laboratories. NRSCs also work together to recruit users by supporting jointly sponsored booths at major scientific conferences in nanoscience, such as the Materials Research Society (MRS) and American Physical Society meetings.

The NSRCs both compete against each other and work together to secure additional DOE funding. Some types of competition include participating in DOE Energy Frontier Research Center and Energy Innovation Hub competitions and advancing DOE priorities in Quantum Information Sciences. These activities reinforce the role the NSRCs play in advancing BES priorities broadly. In addition, there are increasing opportunities for the NSRCs to partner to respond to open scientific research calls and be more strategic in responding to national scientific needs. The collective response to the COVID-19 pandemic showed how the extant capabilities and expertise could be applied immediately and innovatively to address a pressing problem. These efforts ranged from CryoEM characterization, virus tagging, development of flow assays, mask characterization, and sensing of viral loads via breath testing. These efforts show the range of areas that fundamental and applied nanoscience capabilities and expertise can impact.

Building on these efforts, the NSRCs are working to enhance synergy across the centers by creating working groups aligned with national needs and DOE priorities. These focus on microelectronics; quantum information sciences; data sciences, artificial intelligence (AI), and machine learning (ML); future pandemics; and clean energy. While this effort is inchoate, it is promising. The ability to clearly articulate how the NSRCs can aid existing communities has the potential to increase facility utilization and impact, steer future decisions on capital and personnel investments, and define future scientific directions more broadly. In addition to the working groups, specific research collaborations have been initiated. The “Electron Distillery” seeks to leverage AI and ML to enhance electron detection via automated processing pipelines, and the “Digital Twin for Spatiotemporal Experiments” integrates experiment, simulation, and data science through AI-enabled information extraction, efficient multifidelity simulations guided by ML, and shared workflows for seamless model-experiment information exchange.

However, there are opportunities to further increase the collective synergy of the NSRCs. It would greatly benefit the user community if there were a single portal for the submission of scientific proposals that would allow access to capabilities at all the centers in a collective fashion. Presently, if a PI wishes to, for example, utilize the scanning tunneling microscopy facilities at the CNM to probe the ultralow temperature response of a material and correlate this with measurements of electronic structure using the angle-resolved photoemission spectroscopy capabilities at the CFN’s x-ray photoemission electron microscopy / low-energy electron microscopy (XPEEM/LEEM) Spectro-Microscopy Endstation at the National Synchrotron Light Source II (NSLS-II), this would require the submission of two separate proposals, two separate user agreements, and two separate user registration processes. There are important and significant structural barriers that make overcoming this challenging, as the user agreement and registration processes are inherently different at the different laboratories; however, a streamlined submission and review process could greatly enhance scientific impact by allowing access to multiple forefront scientific capabilities. It is also important to note that coordinated proposals of this type would require increased funding from users to allow travel to multiple locations, though the increase in remote access facility usage could alleviate this problem to an extent.

Currently, there are mechanisms for personnel and cross-laboratory knowledge exchange. These activities include involvement in user workshops, invitations to present at these workshops and at dedicated seminars, cross-facility usage by staff, and participation on review panels for other NSRCs. Furthering this through a sabbatical program could deepen ties across the centers, facilitate knowledge exchange, and provide opportunities for NSRC staff to reinvigorate their research programs in the same way that tenured faculty do in academia.

Additionally, there are existing efforts between the centers regarding topics such as shared software facilities, data management, and data exchange. This is an area of high importance to the international scientific enterprise. Because of their size, scope, funding levels, and funding stability, NSRCs have a unique opportunity to lead in these areas, collaborating with other larger DOE efforts (Hubs, Energy Frontier Research Centers) and affiliated materials research efforts in other agencies (e.g., NSF Materials Research Science and Engineering Centers, Science and Technology Centers, and Engineering Research Center) and data sharing efforts such as the Materials Research Data Alliance.

It is recommended that the centers develop a comprehensive, cross-center strategic plan, that focuses on how their collective efforts could be best positioned to meet national science priorities and scientific grand challenges. The centers could convene a strategic planning committee with representation from all five NSRCs as well as external scientific leaders. This committee should identify three to five priority research areas (these may or may not be aligned with the working group topics identified above), where the NSRCs are well-positioned to have a significant impact through collaboration. For each priority area, the committee could develop 5-year roadmaps outlining specific goals, needed instrumentation and infrastructure development, data management and analysis plans, and community engagement efforts.

To further facilitate this collaborative effort, the NSRCs should hold regular joint workshops and retreats focused on the developed strategic priority areas. Seed funding should be made available for initiating multicenter research projects, and funding incentives should be put in place to encourage NSRC staff scientists to actively participate in collaborative efforts between centers.

A set of metrics should be developed to track the success of strategic priorities and collaboration efforts. These could include new multi-investigator and multicenter publications, adoption of co-developed instrumentation by the scientific community, use of shared data infrastructure, and examples of policy impacts enabled by NSRC collaboration. Annual reviews of progress should inform ongoing strategic planning.

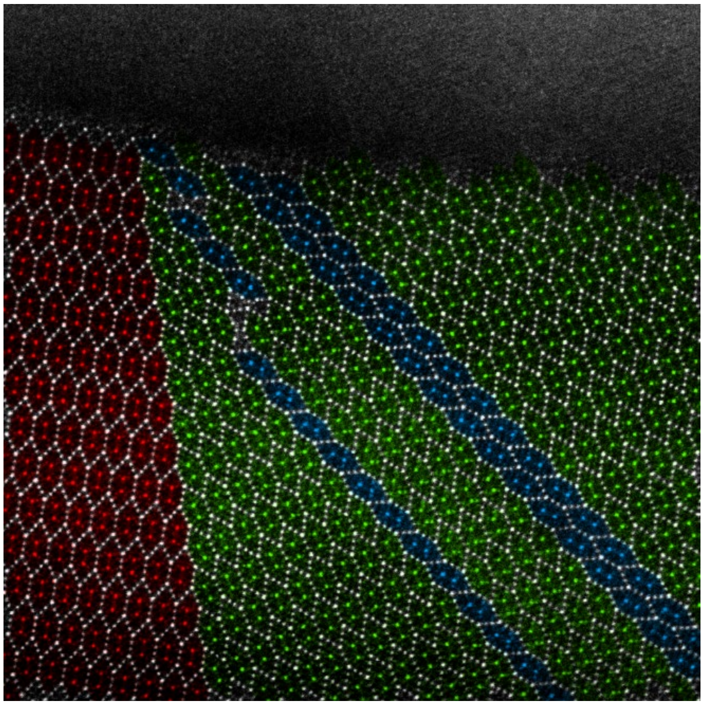
The NSRCs have demonstrated remarkable individual success since their inception, but the future demands increased cooperation to tackle complex scientific challenges. A singular strategic vision can unleash their full potential impact.

HIGHLIGHT 6: COLLABORATION ACROSS NSRCS

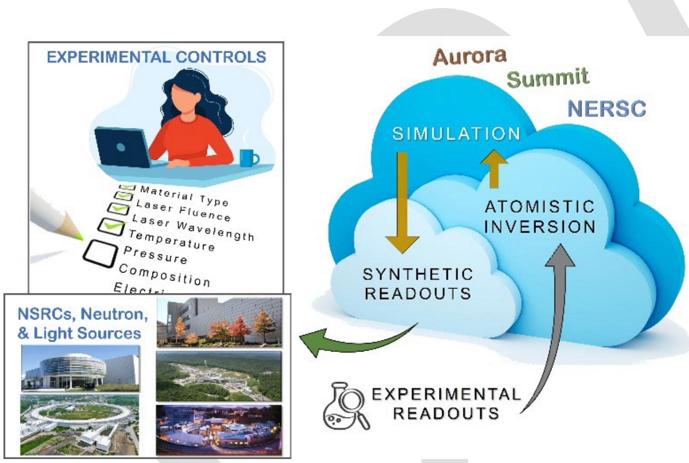
While the NSRCs have unique areas of expertise, they also maintain complementary capabilities. With cooperative effort, these commonalities and differences can be leveraged to advance scientific development in key areas. Two examples of these efforts include development of advanced microscopy capabilities and active work in creating digital twins for NSRC resources.

Transmission electron microscopy development

Transmission electron microscopy (TEM) is a core characterization tool used broadly across materials science, chemistry, biological sciences, and other disciplines. Despite the current ubiquity of basic imaging, many researchers are actively pursuing new capabilities and advances in TEM. The NSRCs have a long history of contributing to microscopy development, with multiple staff having received awards (e.g., Microscopy Today Innovation Awards, the Microscopy Society of America's Burton Medal, R&D100 awards, and DOE Early Career Research Program awards). Work across the NSRCs is pushing the limits of resolution, both in space and time. Researchers have extended atomic resolution microscopy from two to three dimensions, integrated synchrotron X-ray and TEM techniques for multimodal characterization, expanded the applicability of cryogenic TEM in materials science, advanced in situ TEM for a broader



Atomic-resolution image of an $Al_{94}Mn_2Be_2Cu_2$ alloy exhibiting superplastic behavior. False color was added to highlight the three primary twin orientations within the field of view (20 nm). Image by Jim Ciston, Colin Ophus, and Boštjan Markoli.



range of environments (liquids, gas pressures, and temperatures) and stimuli (electrical biasing, electrochemical, and mechanical), and brought electron microscopy to ultrafast timescales. The innovations will only continue, with new detector and data processing technologies, including those developed by the NSRCs, accelerating what is possible. Specializing in different state-of-the-art TEM techniques enables the NSRCs to maintain consistent, baseline capabilities while developing distinct strengths.

Digital twin project

The NSRCs house world-class instrumentation that can characterize materials across many orders of magnitude in time and space. These instruments have both limited capacity and high demand from users. Given the constraints on resource allocation, users are generally restricted in the number of experiments they can reasonably perform given the available instrument time. To help maximize the impact of instrument time, a collaborative effort among the NSRCs to develop digital twins to represent the spatiotemporally resolved experiments is underway. Through this digital twin system, users can test out various experimental controls to perform optimizations without consuming instrument time. An initial version has been developed that allows users to access readouts highlighting potential physics or phenomena of interest for further exploration in actual experiments. As the usage of this model increases, so does its accuracy as the additional data feeds into the ML model and aids in its training. Work on the next iteration of the digital twin is ongoing.

SECTION 4

Synergy between Nanoscience Research Centers and other User Facilities

Based on DOE's initial vision for synergy with other user facilities, four NSRCs are co-located with large-scale facilities such as synchrotron or neutron, and high-performance computing (HPC) centers. CINT gains its synergy by working with several materials and characterization laboratories at both SNL and LANL.

The missions of NSRCs, as user facilities, include characterization, synthesis, nanofabrication, and computation. The most logical synergetic areas are characterization (with synchrotron and neutron facilities) and computation (with HPC facilities). Over the years, collaborating with other user facilities has greatly enhanced the impact and visibility of NSRCs through new user programs, new capabilities, and new sciences.

The co-location is important even in the age of modern communication and high-speed internet connectivity. While many interactions with the NSRCs, including complex experiments, can be accomplished virtually, meeting in person is still indispensable for collaborative research involving brainstorming and in-depth discussion. Novel ideas and breakthroughs often arise serendipitously when people of different backgrounds and expertise have opportunities to mingle in person.

The synergy in characterization is rooted in the complementary nature between the techniques involved. Electron microscopic tools at NSRCs could achieve atomic resolution, whereas many synchrotron and neutron methods measure averaged microstructure of bulk materials. Combining both capabilities would allow multimodal measurement of the same materials over a wider length scale. Time-resolved in situ or operando measurements could be readily carried out using synchrotron X-rays, especially for bulk materials at various external environments; but we might still need ex situ microscopic tools at NSRCs to supplement microstructure details at selected conditions to achieve better understanding.

In addition, expertise at NSRCs in manipulating miniature samples with precision could be transferred to light sources when smaller beam spots become prevalent after upgrades. Co-developed beamlines or having an NSRC-developed instrument at the beamline can benefit users greatly, as user experience is largely dependent on what's available for sample handling, sample environment, instrument control, and data processing. Lastly, new sciences could emerge by replacing electron excitation with X-ray excitation on commercial instruments as shown in Highlight 7. NSRCs have roles to play for each of these.

Working with HPC centers (the Argonne Leadership Computing Facility [ALCF], the Oak Ridge Leadership Computing Facility [OCLF], and the National Energy Research Scientific Computing Center [NERSC] at Berkeley) is another synergetic area. Large-scale computation has become ever more demanding in recent years with the advent and rapid development of ML and AI. Having access to the most advanced characterization and most powerful computation tools at the same campus is one of the greatest advantages for co-located user facilities. *The whole is truly greater than the sum of its parts.*

The following four examples showcase the scientific impact of synergy between NSRCs and other user facilities.

Differentiating metallic speciation at atomic resolution. By combining scanning tunneling microscopy with synchrotron excitation, absorption spectra from the L2,3 and M4,5 absorption edge of iron and terbium single atoms were observed at the Advanced Photon Source (APS) 4-ID-E beamline, the world's first synchrotron X-ray scanning tunneling microscopy beamline. In this multimodal system, co-developed by **CNM and APS**, electrons were resonantly extracted from single atoms in close proximity (<0.5 nm) to the scanning tunneling microscope tip. Such an experiment is not possible with conventional scanning tunneling microscopy.[9]

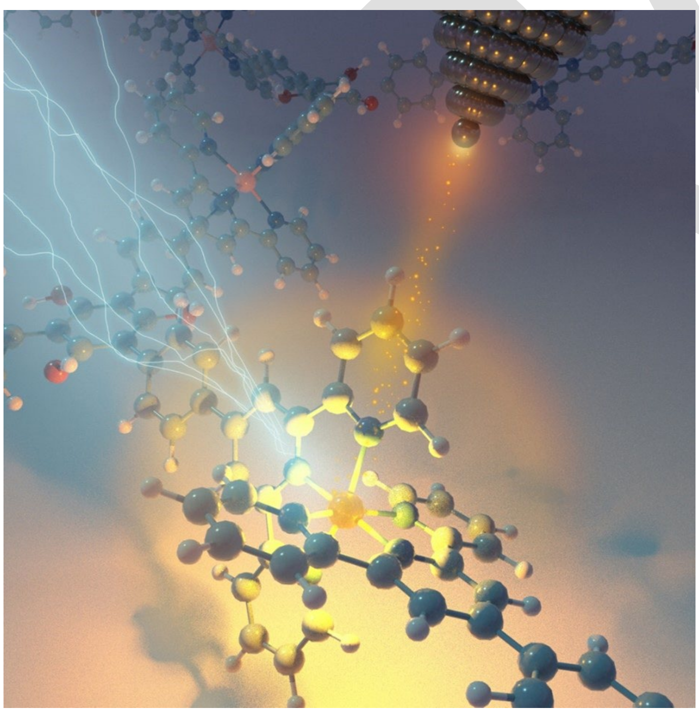
Determination of Ir oxidation state in iridium dioxide films is key to understanding strain-controlled growth of thin IrO_2 oxide films. At **CFN**'s XPEEM/LEEM beamline at **NSLS-II**, the evolution of the Ir oxidation state during film growth, as well as local crystallinity and composition, were monitored using micro-spot X-ray photoemission (μXPS) spectra from the Ir-4f core level. This work is critical for making high-quality metal oxide films on "stubborn" metals like iridium or ruthenium which are difficult to oxidize.[10]

The **interaction potential in a colloidal suspension** system was determined by combined use of small angle neutron scattering at Spallation Neutron Source (SNS) and ML, which circumvents the efficiency-accuracy tradeoff. The molecular-dynamics-based digital simulation was performed by CNMS at OCLF, which trains Gaussian process regression for inverting the scattering structure factor S(q) to obtain the effective interaction.[11]

Deep learning simulation of crystal structure factors from electron diffraction patterns with multiple scattering. Strain maps with high accuracy and spatial resolutions could be obtained from scanning electron nanodiffraction. This technique, however, is limited due to multiple scattering. Researchers from CNM and TMF solved this problem by implementing a Fourier space, complex-valued deep-neural network, FCU-Net. The network was trained using over 200,000 unique simulated dynamical diffraction patterns from different combinations of crystal structures, orientations, thicknesses, and microscope parameters, which are augmented with experimental artifacts, using NERSC under the Materials Project.[12]

HIGHLIGHT 7: COLLABORATION WITH LARGE FACILITIES: CNM AND THE ADVANCED PHOTON SOURCE

Using Two Facilities to Characterize Single Atoms



Combining capabilities from two specialized facilities enabled researchers to study single atoms via X-rays for the first time. *Image by Argonne National Laboratory.*

The Nanoscale Science Research Centers do not operate in isolation. While all are located at DOE national laboratories, most are also co-located with other large-scale user facilities. This provides unique opportunities for collaboration by leveraging multiple leading-edge or highly specialized capabilities.

Researchers using synchrotron light sources, like those at the Advanced Photon Source, have been able to measure extremely small samples down to the nanoscale. However, those samples still contain around 10,000 atoms. Increasing the resolution to the level of individual atoms has proven extremely challenging. This has been overcome through a large, combined effort between the Advanced Photon Source and CNM that enabled researchers to study single atoms by combining X-ray methods with scanning tunneling microscopy for the first time. The novel beamline included a customized scanning tunneling microscope to measure the electrons emitted from individual atoms that are excited by synchrotron X-rays. This produced a characteristic fingerprint for each individual element in a sample. Beyond simple fingerprinting, the spectrum provided information about the atom's chemical state similar to traditional X-ray adsorption studies of bulk materials.

The team studied systems where a single metal atom was isolated from others of the same element in a molecular host. This allowed the researchers to measure the signal from one specific atom in a known position. The study demonstrated the applicability of the method to both iron and terbium, highlighting the elemental flexibility of the technique. The results represent an unprecedented level of resolution for X-ray analysis and pave the way for future fundamental science discoveries.

Ajayi *et al., Nature,* **618,** 69–73 (2023). [DOI: 10.1038/s41586-023-06011-w]

In addition to high-impact publications, NSRCs have worked with synchrotron sources through (1) partner user programs, (2) co-development of beamlines, and (3) co-developed instruments at endstations. Some examples are as follows:

- Partner user programs between CFN and NSLS-II at the complex materials scattering (CMS) and soft matter interface (SMI) beamlines. These programs enable high-throughput exploratory small-angle X-ray scattering (SAXS)/wide-angle X-ray scattering (WAXS), high-flux resonant SAXS/WAXS, and advanced capabilities for autonomous material discovery.
- CFN facilities at two NSLS-II beamlines: an XPEEM/LEEM facility at the electron spectro-microscopy (ESM) beamline and a three-dimensional X-ray nanoscale coherent imaging facility at the hard X-ray nanoprobe (HXN) beamline. The XPEEM/LEEM facility is unique in the United States for chemical, electronic, and magnetic characterization with nanometer-scale resolution.
- Rheo-SAXS-X-ray photon correlation spectroscopy (XPCS) (APS 8-ID-I): Study of nonequilibrium dynamics of complex fluids under shear and energy dissipation by combining rheological measurement with SAXS and XPCS (CNM and APS).
- 4D nanoprobe as part of the APS-Upgrade project (CNM and APS).
- Real-time inversion on X-ray nano ptychography data streamed directly from a detector at up to 2 kHz at the APS HXN beamline 26-ID-C, accomplished through an edge deployment of a neural network algorithm trained with ALCF HPC resources. This nano-ptychography capability can image strain, polarization, or crystallographic phases in response to mechanical, optical, or electrical stimulus (CNM, APS, ALCF).
- TMF has developed both hardware and software for the Advanced Light Source (ALS), including a state-of-the-art sample delivery system, and *Scope Foundry*, an instrumentation and control development for ALS endstations.

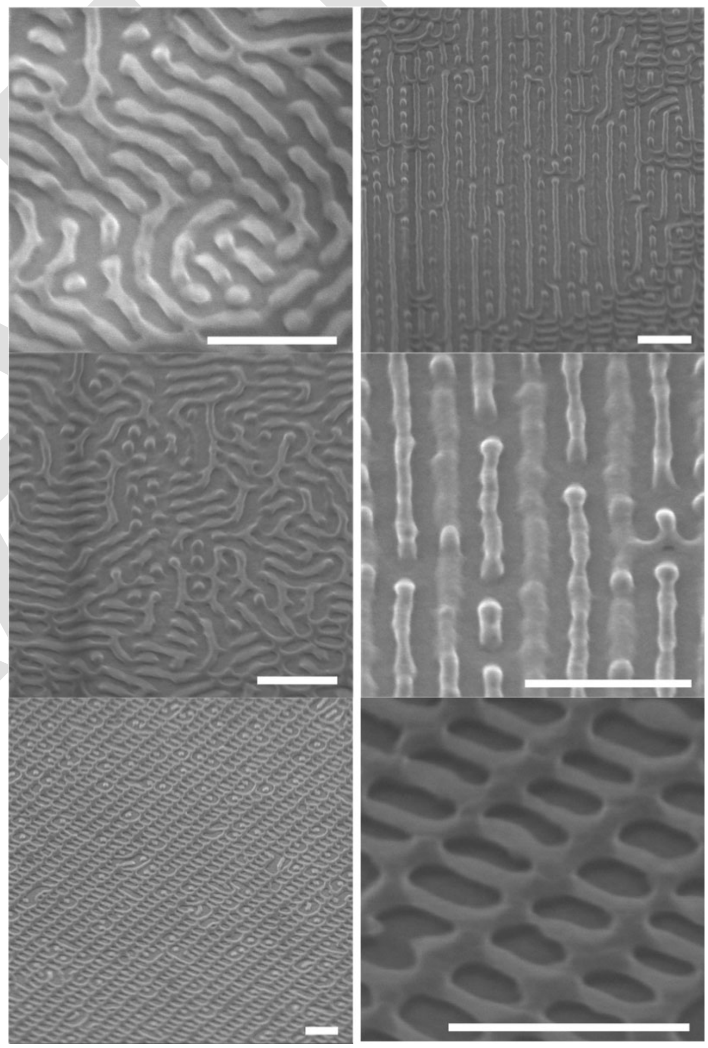
RECOMMENDATIONS

Develop advanced capabilities in conjunction with upgrades at synchrotron and neutron facilities. There are waves of upgrades at various synchrotron and neutron facilities including APS-U, ALS-U, NEXT-III, and Second Target Station at SNS. As these upgrades mostly focus on the sources and frontend, there are gaps to fill for instrumentation inside the endstations. This is because capabilities of a beamline and user experience are largely shaped by the sample handling system, sample environment cell, and data analysis at the endstation. NSRCs are in a unique position to work with synchrotron and neutron sources in these areas.

Develop unique capabilities at NSRCs including leveraging with co-located user facilities. Unlike large-scale facilities, which are unique, NSRCs may face competition from other laboratory-based user facilities (such as those sponsored by NSF) and university labs. Free of charge for open research is certainly attractive, but the need for proposals and for users to work away from their home institutions could be a drawback. When a facility is unique, however, travel and other expenses might become secondary, as shown by strong user demands at various light sources. There may be several ways to achieve uniqueness: (1) have more user programs at the co-located synchrotron or neutron source; (2) develop customized sample environments to achieve high temperature, pressure, or other in-situ or in-operando conditions, as additions to commercially available instruments; and (3) develop customized, one-of-a-kind capability for a particular research area with unmet demands and when such capabilities are not available commercially.

HIGHLIGHT 8: LOOKING TOWARD THE FUTURE: ARTIFICIAL INTELLIGENCE, AUTOMATION, AND DATA

As science continues to move forward, researchers must engage with an ever-changing landscape of digital-based tools. The advent of modern computing has enabled scientists to produce, store, and share vast quantities of data that may already hold key insights into urgent problems. Finding ways to effectively use these data, as well as emerging analysis techniques, represents a challenge across all fields of science. This is particularly relevant for facilities like the NSRCs, where advanced instrumentation leads to massive amounts of data.



Scanning-electron microscopy images of new nanostructures discovered using AI to lead autonomous experiments. All scale bars represent 200 nm. *Image by the Center for Functional Nanomaterials (CFN).*

Researchers are implementing rapidly evolving AI/ML algorithms to enable data-driven discovery. Projects across the NSRCs are taking AI/ML techniques and applying them to synthetic and theoretical problems. For example, work at the (Center for Functional Nanomaterials) CFN used an AI-enabled autonomous X-ray scattering technique implemented at the co-located NSLS II to discover new nanostructures that emerge in mixtures of self-assembling materials. Discovering these nanostructures using traditional research methods would be significantly slower and more challenging given the very complex parameter space of multicomponent self-assembly.

The team used an autonomous system that integrates AI/ML decision making into real-time experimentation. By directing measurements to search for novelty while exploring the parameter space of the sample, the AI-enabled experiment identified three novel, previously unreported polymer structures in only six hours of data collection. The approach applied to discovering these new, complex structures is flexible and could pave the way for additional discoveries relevant to clean energy and microelectronics. By speeding up the materials discovery loop, researchers can solve more challenging and complex problems in less time.

Doerk *et al*., *Science Advances,* **9**, eadd3687 (2023). [DOI: 10.1126/sciadv.add3687]

SECTION 5

Best Practices for a Diverse User Community

The NSRCs have a strong emphasis on mentorship and knowledge sharing with the broader scientific community. Maintaining a diverse user base is therefore a key component of an effective NSRC. The development of best practices to cultivate a diverse user base requires consideration of mechanisms to engage a broad set of users and track their participation and outcomes.

The NSRCs actively track the institution type of user projects that are classified as academic, industry, or government lab. Academic users can be further divided into their institution type such as Carnegie Classification Research 1 (R1) institutions, non-R1 institutions, MSIs, and ERIs. User diversity may also take into consideration the geographic location of the user institution (with special awareness of EPSCoR jurisdictions); specific demographics of individual users such as gender, ethnicity, race, and sexual identity/orientation; and the stage of their career (graduate student, postdoctoral scholar, early career faculty, etc.). The NSRCs have detailed information on the institution type of users but have not historically tracked information on individual user demographics and career stage.

In FY 2023, the majority (55%) of projects were from users at U.S. academic institutions and 27% were local users at the host laboratory. Researchers affiliated with MSIs were active users of the NSRCs, representing an impressive 32% of all proposals from U.S. academic institutions, with good conversion of successful MSI proposals to publications. The participating MSIs tend to be regionally located near an NSRC in the Southwest and West. While the MSI participation is significant, it was noted that many of these proposals come from a small group of R1 institutions. For example, in FY 2022, 151 out of 549 user proposals (27.5%) were from the University of California at Berkeley, a recently designated Asian American and Native American Pacific Islander (AANAPISI) institution located near TMF. Another example is the University of New Mexico, a Hispanic Serving Institution (HSI) near CINT which submitted 75 user proposals (13.7%) in FY 2022. A much smaller number of proposals (11 in FY 2022, ~2%) were from Historically Black Colleges and Universities (HBCUs) or Predominantly Black Institutions (PBIs). The majority of HBCUs and PBIs are located geographically away from the NSRCs, which presents a barrier to participation.

The centers have put in place programs to engage diverse communities and better understand how to serve their needs. For example, the NSRCs are doing targeted outreach at professional society meetings to recruit both users and new staff members. Another approach is to increase remote access to facilities to make it easier for researchers at geographically distributed MSIs to participate. The DOE Workforce Development for Teachers and Scientists (WDTS) Visiting Faculty Program has been instrumental in bringing in users from MSIs, which has led to successful outcomes. For example, CFN user Professor Armando Rua from the University of Puerto Rico at Mayaguez recently received a large grant from the Moore Foundation which expands upon the work he initiated under the DOE-WDTS Visiting Faculty Program. The CINT Core Summer Research Program has also been very successful in bringing students from MSIs for summer research experiences. Another strategy being used is to partner with R1 institutions that have relationships with regional MSIs as a way to broaden participation.
The NSRCs provided user data from four centers, CFN, CNM, CNMS and the MF, and the data can be considered representative of all six centers. Centers reported that 22–25% of users at these facilities identify as female. Across these four centers, researchers 20–29 years of age accounted for 34% of users and those 30–39 years of age accounted for 36% of users (from those who self-identified). This relatively youthful user group offers an untapped opportunity to diversify the NSRCs. For example, in the physical sciences and science technologies fields, 34% of doctoral degrees awarded in 2017–2018 went to women. In the engineering and engineering technologies fields, 24% were awarded to women (National Center for Education Statistics). The NSRCs are thus falling somewhat short relative to the proportion of female graduate students in science, technology, engineering, and

math (STEM) fields. Additionally, while 'access of any and all abilities' was articulated as a goal, no actions are taken to reflect this goal beyond compliance with the Americans with Disabilities Act of 1990.

The NSRCs are well positioned to reach students even earlier in the pipeline than those who participate in the user program. The centers are engaged in an impressive array of student internship programs, from the DOE Office of Environmental Management MSI Partnership Program internships at SNL/LANL CINT, and ANL CNM for undergraduates at MSIs, to the Brookhaven National Laboratory Student Partnerships for Advanced Research and Knowledge for high school students and the DOE Community College Internship program at ORNL CNMS.

HIGHLIGHT 9: ENGAGING A DIVERSE USER COMMUNITY

The user community is the customer and essential to the success of the NSRCs, often collaborating with staff to find answers to challenging scientific questions. The centers are working to broaden their impact by finding new ways to engage with diverse communities. Effectively accessing NSRC resources requires knowledge of the proposal process and the different capabilities available across the NSRCs. One route to addressing these challenges is national outreach to professional societies and other specific groups.

Scientist Suji Park shows the Quantum Material Press to a group of scientists attending a recent workshop at Brookhaven National Laboratory co-organized by CFN, the Brookhaven Diversity, Equity, and Inclusion office, and the Interdisciplinary Consortium for Research and Educational Access in Science and Engineering (InCREASE). InCREASE is a consortium of universities whose mission is to promote research and education in Minority-Serving Institutions. *Photo credit Brookhaven National Laboratory.*

The NSRCs are participating in conferences that bring together researchers from underrepresented communities. Through outreach efforts at meetings of the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, the National Society of Black Physicists, the Society for Advancement of Chicanos/Hispanics and Native Americans in Science, and the Society of Women Engineers, the NSRCs—as individual entities and collectively—are creating connections with a broader user base. These efforts dovetail with more targeted programs hosted by the centers that provide internships and support in proposal writing for potential users across the United States.

The NSRCs have an outsized effect on colleges and universities in their region. This significant regional influence provides opportunities for relatively broad engagement geographically, but still has limits. Travel can be a significant challenge for users from further afield, particularly if they work at resource-constrained institutions. The NSRCs, like other Office of Science user facilities, are helping to mitigate this challenge through greater use of remote access capabilities that were developed or refined in response to the COVID-19 pandemic. These virtual opportunities enable users to leverage NSRC knowledge and instrumentation without requiring travel, and open the door to users who would have previously been unable to engage with the NSRCs.

STAFF

It is recognized that increasing the diversity of NSRC staff helps to promote the participation of diverse users. The NSRCs have worked to develop transparent goals for staff recruiting and sharing of best practices, which has resulted in increased diversity of recent hires. For example, the majority of recent hires at CNM have been women and members of underrepresented groups, and a significant fraction of staff (36%) at CFN and TMF are women. The NSRCs articulated an effort to assess the research culture through user surveys. Surveys demonstrated user satisfaction with the excellent staff and some concerns about outdated facilities and the cost of travel. It is unclear whether the research culture was assessed.

Moving forward, the NSRCs must considerably expand their proactive efforts to increase the diversity of their user community and their staff. Their recent efforts at targeted recruitment at professional societies, remote equipment access, visiting faculty positions, and summer research internships have been effective but should be further expanded to include an emphasis on training. For example, summer schools and short courses can be an effective mechanism to bring diverse users to the centers, thereby lowering the barriers to entry. The centers should work toward development of metrics to assess the effectiveness of these various efforts that are reasonable and achievable.

INDUSTRY

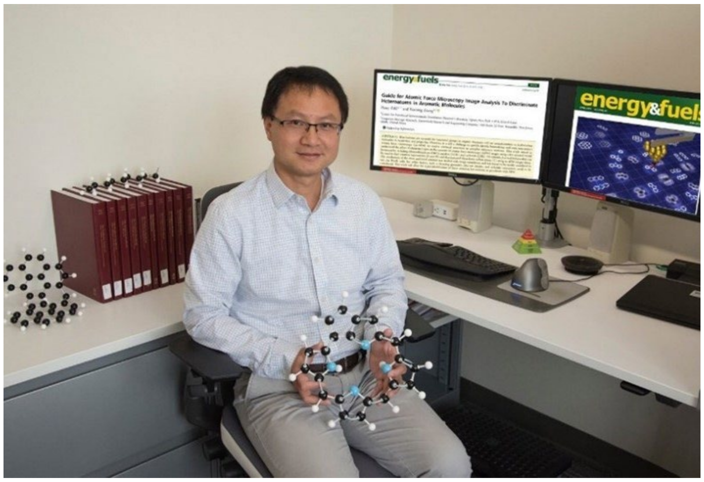
Industry participation in the NSRCs is relatively low (~6% of users in FY 2023). It was noted that the national labs themselves have significant industry interaction, but attracting industrial users to the NSRCs has been a challenge due to the need to have collaborative research agreements in place which can take significant time. While engaging with industry does not directly (if at all) address national priorities in ensuring equitable access to educational and research resources across demographic groups, industry participation is important as it provides a vehicle to educate staff scientists on commercially relevant problems. Anticipated impact on the national economy was articulated, but evidence of the connection is lacking. The NSRCs have been very effective in connecting with small companies associated with technology spinoffs, but engagement with larger companies has been limited.

Strategies to increase industry engagement include increasing industry participation on proposal review committees, executive/scientific advisory committees and partnering on DOE programs that support industry research such as DOE technology offices, Technologist in Residence, etc. CINT, for example, has included plenary speakers from industry in their last two annual user meetings. The centers are encouraged to continue engaging on industry-relevant science challenges and increase industry participation via short courses, summer schools, and invited seminars. There is also interest in pursuing an NSRC-wide operating model and industry user agreement to lower the barrier for collaboration and responsiveness. One great example of industry-NSRC collaborations is in instrument development, for example the microscope, specimen stages, and detectors associated with the TEAM project led to significant commercial innovations that have greatly benefitted the international transmission electron microscopy community.

INTERNATIONAL USERS

Diversity within the context of international participants was also discussed. Around 9% of users are affiliated with international institutions primarily located in Europe and Asia. There are opportunities to engage more broadly, particularly with the global south (e.g., South America, Africa, Southern Asia). While individual researchers have made some efforts in this area, a more collective effort could be beneficial to provide more diverse representation to reduce unconscious bias. There is also value in engaging international scientists for recruiting and goodwill.

HIGHLIGHT 10: CONNECTING WITH INDUSTRIAL PARTNERS



Since 2008, ExxonMobil chemist Yunlong Zhang has been a CFN user, collaborating to use high-resolution atomic force microscopy to study petroleum chemistry and develop a “guide” for discriminating pollutant-causing sulfur and nitrogen atoms in petroleum mixtures. *Photo credit Yunlong Zhang, ExxonMobil.*

While academic institutions represent the largest fraction of the NSRC user base, collaborations with industrial partners represent important opportunities for innovation. Like their academic counterparts, industrial users—from small startups to large corporations—require the specialized instrumentation and resources at the NSRCs to advance their research objectives. Each NSRC has individual, successful collaborations with industrial users across a vast range of nanomaterial applications.

From developing the synthesis protocol for a precision nanoparticle platform for breast cancer detection at CINT to creating an environmentally friendly solid lubricant based on graphene at CNM, the innovative technologies emerging from NSRC-industry partnerships take fundamental science knowledge and apply it to pressing challenges. Another example is the CNMS contribution to process development and fabrication of devices used in protein bioelectronics in collaboration with a startup company. Projects such as these have resulted in awards, patents, and funding from both government programs and private capital.

These collaborations rely on the distinct expertise and capabilities of the different NSRCs. X-therma, a longtime industrial user of the MF, is developing a cryopreservative based on peptoids. The MF has a suite of tools designed for synthesizing, purifying, and characterizing bioinspired polymers such as peptoids that would be inaccessible to a startup company on its own. Similarly, the unique, low-temperature, noncontact atomic force microscopy capabilities at CFN have led to an extended collaboration with users from ExxonMobil, providing them with unique insights into the interactions between catalysts and the heteroatom pollutants found in petroleum molecules, such as sulfur and nitrogen, in pursuit of production of cleaner fuels and products. These types of highly specialized instrumentation provide opportunities for meaningful collaboration with industry.

SECTION 6

Future Directions

Moving into the future, the NSRCs have an opportunity to inform and empower the next generation of nanoscale science and materials research. As a true national resource, the NSRCs collectively provide potential competitive advantages for the nation in terms of materials design and synthesis, capability development, workforce development, and data generation. The future directions of the NSRCs, individually and (more impactfully) together as a resource, will undoubtedly affect the directions and impacts of nanoscale science for the nation and the world. Readiness and agility to pivot to emerging areas of national need such as quantum information science, microelectronics, biopreparedness, or clean energy is essential for maximum impact. A readiness to deploy in individual and concerted efforts is essential, creating and sustaining unique capabilities to address priority science.

The NSRCs are building the next generation of scientific leaders as well as scientists who excel in the support of the user communities critical to the success of the centers. By maintaining and supporting this flexible mindset approach to teaming, which is essential in today's dynamic research ecosystem, the NSRCs have the opportunity to assume an augmented role in training our future scientific leaders and highly skilled workforce. They should, as a group, consider NSRC-specific internships and work/study programs, leveraging ongoing and new connections to previously underserved populations within the STEM fields. An opportunity for close partnering between components of the Office of Science (i.e., BES and WDTS) could facilitate success. From an international competitiveness perspective, the centers have the potential to significantly improve the U.S. situation through expansion of access to advanced instrumentation, and through increasing the number of trained personnel who can use state-of-the-art capabilities to advance U.S. competitiveness in science and industry.

Undoubtedly, the NSRCs will expand their roles in instrumentation development. NSRCs can position themselves to play a more significant role by tackling some of the well-understood data problems and ultimately providing a nanoscale science Public Reusable Research data resource. The centers already provide a massive source of data on a wide range of topics/materials in a unique way. While some level of infrastructure and staff thinking about these critical issues already exists, future opportunities are almost boundless.

The NSRCs will continue to invest in directions defined by individual centers, but they are also well-suited to tackle ambitious challenges together. In one area of potential synergism, they could work toward support of competitive proposals for inter-NSRC collaborations. The centers have a strong track record of pivoting to new topics and developing new capabilities to meet highly challenging problems emerging from science outside of the NSRCs, leveraging user input and internal research. One example is the quantum press (QPress) developed at the CFN (see Highlight 11).

One compelling case for synergy is developing autonomous methods in materials science taking advantage of high-speed computing capabilities. Autonomous experimentation is about how science is done rather than the science itself. The autonomous approach is innovative and should be couched in the scientific context of the need for this approach. Part of the excitement of the autonomous methods is how it can help make science more efficient, for example when applied to materials discovery. To implement any new program, for example in autonomous experimentation, individual centers must leverage their own discretionary investments with collective activities that are highly synergistic.

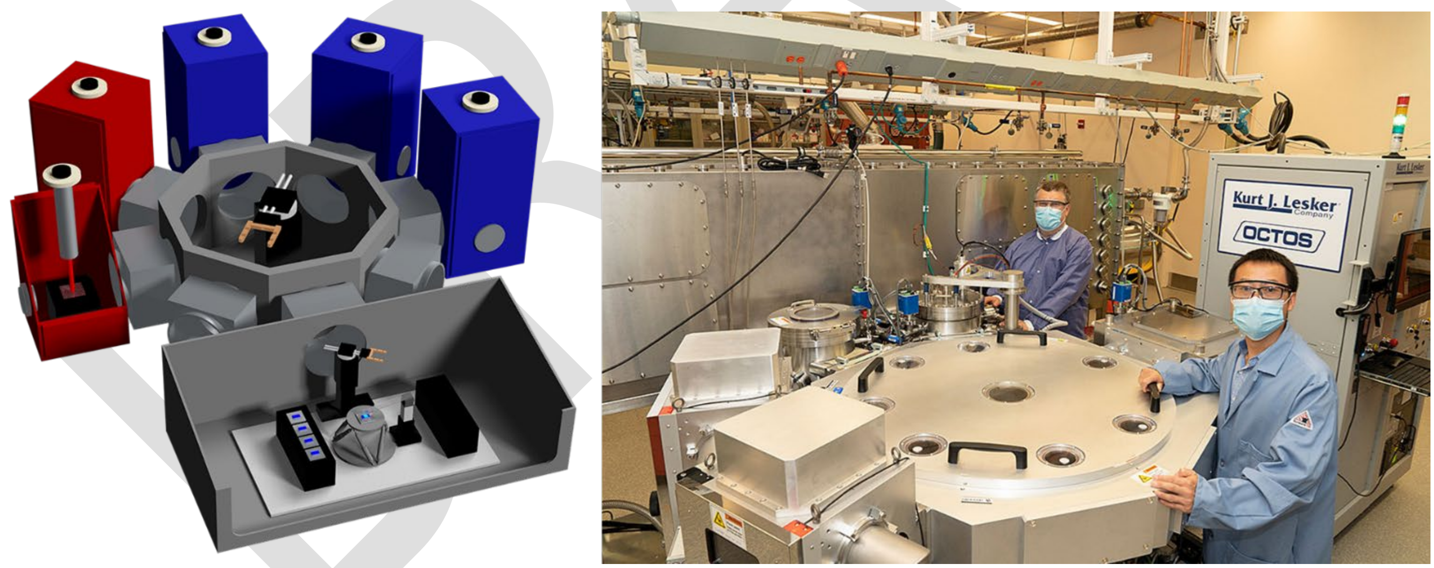
To increase the ease of user access, we endorse the enhancement of the current website for all of the centers to form a portal with information about all the NSRCs that would make it easier for users to access the resources of the different centers. This would lead to an interconnected network of centers with integrated infrastructure. Improving the simplicity of multiple center proposals would be equally impactful, but involves cooperating on legal, contractual, and other issues outside the control of the NSRCs. This could be leveraged through its relevance to large user facility proposals where there is a universal proposal system that DOE has supported implementing at the light sources. In this instance, remote access is seen as a way to leverage the user community, especially in historically underrepresented institutions, and should be strengthened.

There should be more holistic strategic planning for the evolution of the centers in very specific directions. It is not reasonable for all NSRCs to move in the same direction, but they need to be complementary. Each center needs to look at their own expertise and see how to pivot to make sure that they are becoming world leaders, but also engage in dialog with the other centers and BES in their strategic decision making.

The NSRC directors collectively identified areas they see as most important for high-impact development: integrating data with experiments including across NSRCs; identifying the next grand challenge in techniques, especially electron microscopy; nanofabrication and microelectronics; and autonomous experimentation. The directors also see potential opportunities in common development of scanning probe microscopy, where most of the centers are active. However, continued awareness and elucidation of the science drivers for all such developments will be critical.

The NSRCs could support common efforts to adapt instrumentation to work in an autonomous way, and develop new software with AI/ML to create a functional system. The integration of multiple capabilities in a single experiment would also be desirable. Programs like this would benefit from a network between staff with detailed knowledge. Such networks have existed informally but could be strengthened.

HIGHLIGHT 11: AUTOMATING QUANTUM MATERIALS PRODUCTION



The Quantum Material Press. *Image courtesy of CFN.*

Beginning with the discovery of graphene, atomically thin, 2D materials have emerged as an exciting area of research, with potential applications ranging from catalysis to quantum computing. While single 2D layers have fascinating emergent properties, their assembly into multilayered structures provides rich opportunities to design new materials with unique electronic, optical, and mechanical properties. The Quantum Material Press (QPress) at CFN is a unique automated facility for accelerating research on 2D materials and layered stacks.

QPress is a one-of-a-kind robotic platform that enables researchers to controllably assemble stacks of 2D layers from a variety of materials, known as heterostructures. The traditional approach to creating these heterostructure materials is highly labor-intensive, requiring hand sorting of hundreds of candidate 2D flakes of the materials. These flakes must then be characterized, confirming their structure and quality, before delicately stacking them to create the heterostructure. This process can take days or even weeks to perform manually.

The modular QPress system robotically moves through a series of synthesis, processing, and characterization stations to greatly streamline 2D heterostructure research. QPress safely stores a searchable repository of candidate 2D flakes in a library for future selection and use. The facility is helping researchers identify new materials for quantum information science, microelectronics, and chemical engineering, among other potential applications. Designed and constructed over a period of three years, the QPress began supporting user research in 2022 and assisted 44 users in 2023.

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Acronyms and Abbreviations

µXPS	micro-spot X-ray photoemission
3D	three-dimensional
AANAPISI	Asian American and Native American Pacific Islander
AI	artificial intelligence
ALCF	Argonne Leadership Computing Facility
ALS	Advanced Light Source
APS	Advanced Photon Source
BES	Basic Energy Sciences
BESAC	Basic Energy Sciences Advisory Committee
CFN	Center for Functional Nanomaterials
CINT	Center for Integrated Nanotechnologies
CMS	complex materials scattering
CNM	Center for Nanoscale Materials
CNMS	Center for Nanophase Materials Sciences
CryoEM	cryogenic electron microscopy
DOE	Department of Energy
EFRC	Energy Frontier Research Center
ERI	Emerging Research Institution
ESM	electron spectro-microscopy
FY	fiscal year
HBCU	Historically Black Colleges and Universities
HPC	high-performance computing
HIS	Hispanic Serving Institution
HXN	hard X-ray nanoprobe
IP	intellectual property
LANL	Los Alamos National Laboratory
LEEM	low-energy electron microscopy
MAS	Microanalysis Society
MF	Molecular Foundry
ML	machine learning
MSA	Microscopy Society of America
MSI	Minority Serving Institution
MRS	Materials Research Society
NERSC	National Energy Research Scientific Computing Center
NNCI	National Nanotechnology Coordinated Infrastructure
NREL	National Renewable Energy Laboratory
NSF	National Science Foundation
NSLS-II	National Synchrotron Light Source II
NSRC	Nanoscale Science Research Center
OCLF	Oak Ridge Leadership Computing Facility
PBI	Predominantly Black Institution
PI	principal investigator
SAXS	small-angle X-ray scattering
SMI	soft matter interface
SNL	Sandia National Laboratories
SNS	Spallation Neutron Source
SSURF	Society for Science at User Research Facilities
STEM	science, technology, engineering, and math
TEAM	transmission electron achromatic microscope
TMS	The Minerals, Metals, and Metallurgical Society
WAXS	wide-angle X-ray scattering
WDTS	Workforce Development for Teachers and Scientists
XPCS	X-ray photon correlation spectroscopy
XPEEM	X-ray photoemission electron microscopy

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