Five-year Strategic Plan

Brookhaven
National Laboratory

Center for Functional
Nanomaterials

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EXECUTIVE SUMMARY

The Center for Functional Nanomaterials (CFN) is a Nanoscale Science Research Center operated for the U.S. Department of Energy (DOE) at Brookhaven National Laboratory (BNL). As a national scientific user facility, the CFN mission is to empower nanoscience research, by providing essential capabilities and technical expertise, achieving breakthrough discoveries through internal research, and swiftly adapting to evolving national research priorities. CFN uniqueness stems from positive synergies among the expert staff, talented facility users, portfolio of distinctive nanoscience instruments, and a core commitment to collaborative research.

The CFN drives nanoscience advances through innovative research methodologies and by supporting cutting-edge capabilities to address complex materials challenges with agility. An adaptable model positions the facility to respond effectively to national research priorities as they emerge. The Five-year Strategic Plan is guided by the ethos of acceleration, embodied in three core nanoscience Themes and two Crosscutting elements, which define a unique CFN identity reflecting the technical expertise of the staff and guiding development of new, state-of-the-art facilities.

The subject of Theme One is *Nanomaterial Synthesis by Assembly*, which envisions design strategies for synthesis of new materials with targeted functionality by assembly of nanoscale components, for rapid explorations of vast landscapes of complex structural motifs. CFN research on self-assembly devises new approaches to interaction- and process-controlled assembly of components, discovers the governing principles underlying self-assembly, and understands assembly pathways using advanced *ex situ* and *in situ* characterization and computational methods.

Efforts are focused on developing nanomaterial synthesis-by-assembly methods and realizing functional material designs from polymer, nanoparticle, biomolecule-based, and 2D material components. Automation of synthesis-by-assembly processes will provide parallelism and reproducibility, facilitate assembly of increasingly complex architectures, provide control of assembly pathways, and allow incorporation of real-time feedback during processing. Advanced characterization and new methods to probe structure include nanoscale coherent X-ray beams at NSLS-II and 3D imaging of nanostructures by cryo- and in-liquid electron microscopy. Theory and simulation complement the experimental effort, including developing effective self-assembly strategies, assessing the inherent stability of resulting morphologies, and mapping the advantages and limitations imposed by kinetics.

The focus of Theme Two is *Accelerated Nanomaterial Discovery*, which seeks to implement artificial intelligence and machine learning to streamline the material synthesis-characterization-analysis loop. While historically the discovery and development of new materials has followed an iterative process of synthesis, measurement, and modeling, suitable integration of advanced characterization, robotics, and machine-learning can potentially radically accelerate this process. The CFN has an established record of discovering nanomaterials by applying new materials synthesis strategies, advanced characterization, and machine-learning. Integrating these efforts will enable autonomous platforms for iteratively exploring material parameter spaces, which have potential to revolutionize materials science by uncovering fundamental links between synthetic pathways, material structure, and functional properties.

CFN scientists are conducting research and developing instruments toward accelerating the material discovery loop. Realizing this vision requires advancing and automating all aspects of the discovery process, including: implementing combinatorial libraries and real-time synthesis platforms; improving multi-modal characterization and analysis of complex datasets; and using machine-learning to drive experiments.

Theme Three emphasizes the study of *Nanomaterials in Operando Conditions*, which accelerates research by monitoring materials in their operating environments. Interrogating materials at the nanoscale to derive atomic-level information on physicochemical processes under operating conditions remains a forefront and evolving nanoscience research field. The CFN will augment its comprehensive suite of instruments for *operando* studies of nanomaterials such as catalysts, photocatalysts, and battery electrodes. The CFN will increasingly integrate *operando* capabilities with data management and computational resources for advanced data analytics.

CFN users, working independently or collaborating with CFN staff, use combinations of *in situ* and *operando* capabilities at high temperatures and variable pressures to understand catalytic reaction mechanisms. Aberration-corrected transmission electron microscopy with high spatial and energy resolution illuminates reaction pathways and structural changes in energy storage systems. Scanned-probe microscopy, infrared reflection absorption spectroscopy, and X-ray photoemission spectroscopy provide details of the elementary reaction steps through coordinated studies of model catalyst systems. Computational methods link atomistic structures to specific spectroscopic signatures and with catalytic functionality.

Two Crosscutting elements increasingly span a majority of CFN research and facility activities. The CFN excels in integrating diverse, complementary capabilities for *Multimodal Nanoscience* investigations, providing a comprehensive toolset to meet the demands of characterizing complex, modern materials. The CFN is also advancing *Artificial Intelligence and Machine Learning for Nanoscience*, developing accessible and robust tools for data processing, instrument operation, and generation of reliable simulation data.

The CFN Strategic Plan is grounded in foundational Pillars of an expert staff, an engaged user community, and a collection of strategic partners — all working safely and supported by excellent operations and a portfolio of state-of-the-art capabilities. The CFN is working toward higher levels of user engagement and diversity, through strategic partnerships with larger initiatives aligned with national initiatives, technical workshops customized to communities with specialized needs, and by visibly promoting user science accomplishments. During the next five years, the CFN will invest in new instrumentation, make major upgrades to distinctive capabilities, and develop new data-analytics and data-management methods to maintain its status as a cutting-edge user facility.

A high priority is continuing to enhance the partnership between CFN and NSLS-II, through: investing further in four partner X-ray nanoscience instruments; working together to identify opportunities to create unique, new capabilities; and advancing joint projects with NSLS-II staff and users that exploit the complementary properties of X-rays and electrons to collect multimodal information on the same samples.

1. MISSION AND VISION

The Center for Functional Nanomaterials (CFN) is a state-of-the-art nanoscience facility with the dual mission of enabling the research of external users and carrying out transformative basic research to discover, understand, and implement nanomaterials. The combination of scientific staff expertise, portfolio of distinctive nanoscience capabilities, engaged community of users, and strong partnership with the National Synchrotron Light Source II (NSLS-II) at BNL, make the CFN unique among nanoscience centers worldwide.

In a modern world with accelerating pace of science and technology advances, the CFN is an essential element of the U.S. research infrastructure, having versatility and nimbleness to respond to research areas of national need. A tightly integrated state-of-the-art nanoscience toolset and deep staff scientific expertise allow CFN users to pursue complex projects involving nanomaterial synthesis/fabrication, advanced characterization, and understanding — all under one roof.

Since beginning operations in 2008, the CFN has become a vibrant hub for nanoscience research, where engaged users and expert staff use the most advanced tools for breakthrough discoveries of new nanoscale materials and phenomena. Deep research partnerships are an important element of CFN operations: e.g., by maximizing the value of co-location with NSLS-II and the complementarity of the two user facilities.

2. INTRODUCTION

In more than sixteen years of nanoscience operations, the CFN has fostered sustained growth of a large, productive community of users who benefit from both the state-of-the-art nanoscience facilities and the scientific expertise of CFN staff. The CFN supported 655 users in 2023, with users continuing to express high satisfaction with their CFN experience. The 2023 survey of user satisfaction indicated that 90 percent of respondents were satisfied with the service provided by CFN staff.

While the CFN user community is both geographically and topically diverse, many user projects cluster around themes addressing key scientific questions and technological challenges. These themes correlate with the distinctive facilities and expertise of CFN scientists. As a result, the CFN has fostered a strong community of user and staff researchers working in pursuit of new understanding in clean energy (catalysis, energy storage), microelectronics, and QIS, among other areas.

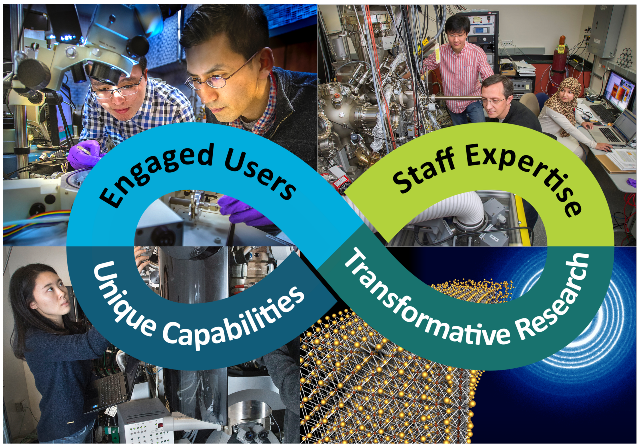


Figure 1. CFN users and expert staff collaborate or work independently, making use of unique capabilities to address complex scientific questions and technological challenges in nanoscience. The staff is recognized for international leadership in DNA-mediated and block copolymer nanomaterial self-assembly, X-ray scattering, and catalysis, among other areas. Advanced CFN capabilities in *operando* probes, aberration-corrected electron microscopes, and robotic synthesis tools stand out.

The CFN operates in a rapidly changing scientific world. For example, recent, intense worldwide interest in quantum information science has increased demand for new synthesis facilities for quantum materials, and advanced characterization capabilities for understanding quantum coherent phenomena. New classes of materials have emerged for this and other applications, such as the expanding palette of ultrathin 2D materials derived from layered van der Waals solids. Heterostructures created from 2D building blocks can possess new types of electronic structure holding promise for quantum information science.

The need for characterizing materials in *operando* continues to grow, for example in efforts to bridge the gap between catalysts operating under industrial conditions and model catalysts probed under idealized conditions. Experiments and instruments are becoming increasingly complex, especially when measurements under variable conditions (*e.g.*, pressure, temperature) are added to those of static parameters. CFN users utilize multiple facilities, including advanced characterization by electron and photon probes. The CFN conducts a focused program of internal research and continually develops new facilities and expertise to take advantage of opportunities, positioning itself as a key facility for accelerating the DOE basic science mission.

Artificial intelligence (AI) and machine learning (ML) are poised to revolutionize the ways that nanoscience research is conducted, and even transform the nature of intellectual work itself. Advancing and implementing methods are central to a CFN facility vision to provide accessible and robust AI/ML tools for data processing, instrument operation, and generation of reliable simulation data with physical constraints.

This Strategic Plan guides CFN actions for the next five years. Progress on the Plan will be gauged using criteria detailed in the Metrics section. Implementing the Plan requires prudently allocating Resources for upgrading facilities, installing new capabilities, and sustaining a world-class staff with the appropriate technical skillsets.

3. OBJECTIVES AND THEMES

The Strategic Plan objectives follow directly from the two-fold CFN mission:

- The CFN is an essential resource for the scientific community, enabling user projects that address fundamental questions and outstanding technical challenges in nanoscience.
- The CFN staff carries out a program of internal research that produces transformative nanoscience breakthroughs.

Mission success rests on the expertise of the CFN staff and the state-of-the-art nanoscience capabilities they develop and operate. Naturally, staff and facilities support a broader range of user nanoscience projects than the narrower scope of the internal research program. However, many projects carried out by CFN users can be grouped into categories that strongly overlap topics underpinning the in-house research program, and which the CFN facilities are well-suited to address. This alignment is very positive and provides an efficient approach to complex, multi-disciplinary science, and ultimately determines the CFN identity.

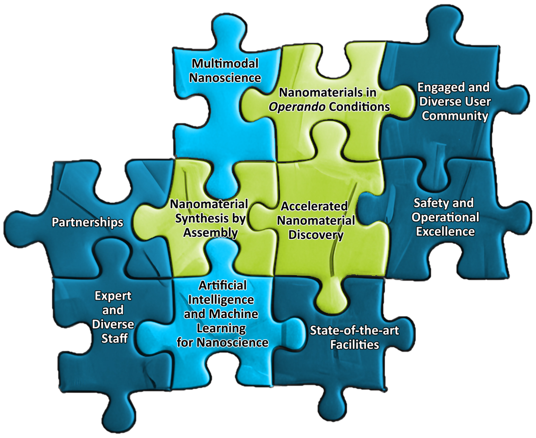


Figure 2. The CFN Strategic Plan is a roadmap for making the CFN an essential resource for the nanoscience community and producing scientific breakthroughs in nanomaterials. Three overarching scientific Themes and two Cross-cutting Directions are supported by five Operational Pillars.

The scientific questions underlying many CFN projects fall under three themes:

- Nanomaterial synthesis by assembly;
- Accelerated nanomaterial discovery; and
- Nanomaterials in *operando* conditions.

These themes utilize the leading expertise of CFN staff in nanomaterial synthesis, block copolymer self-assembly, and DNA-mediated nanostructures. They uniquely leverage the CFN capabilities for *in situ* imaging and spectroscopy, and X-ray based techniques both at the CFN and NSLS-II.

Two cross-cutting themes underlie many activities being pursued throughout the CFN:

- Multimodal Nanoscience; and
- Artificial Intelligence and Machine Learning for Nanoscience.

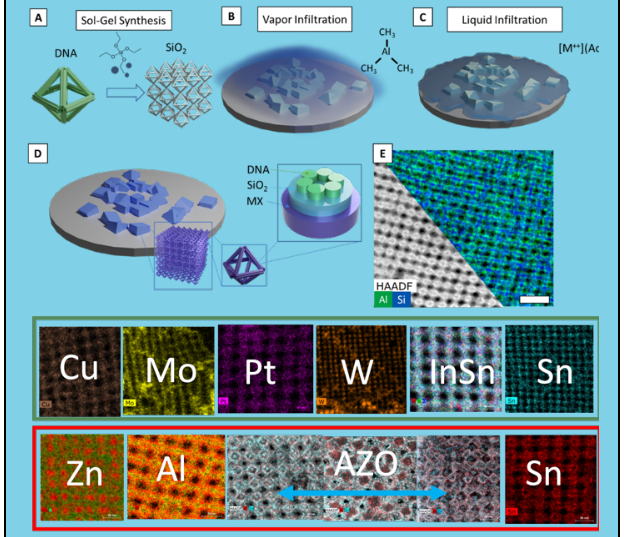
Successful development of these themes rests on five sustaining Pillars, which are:

- Conducting research with Safety and Operational Excellence;
- Hiring and mentoring an Expert and Diverse Staff;
- Fostering and supporting an Engaged and Diverse User Community;
- Providing State-of-the-art Facilities for nanoscience; and
- Engaging in Partnerships for broadest impact.

3.1 Theme 1: Nanomaterial Synthesis by Assembly

CFN fundamental research into nanomaterial synthesis by assembly is important to national initiatives such as microelectronics, advanced manufacturing, and clean energy (**Sidebar**). This theme encompasses self-assembly, traditional nanofabrication, emerging processing methods such as additive manufacturing, and integration of ‘top-down’ and ‘bottom-up’ methods. Chemical and biological synthesis advances have generated a wide palette of structurally diverse and property-specific nanoscale components, including tailored polymers and supramolecular complexes, designed proteins and DNA nano-objects, and shaped nanoparticles. This material toolkit affords a rich opportunity to create a new nanomaterial synthesis paradigm with multiscale and multimaterial control through *by-design* assembly of components into targeted larger-scale functional architectures. Longstanding CFN research in self-assembly (Figure 3) develops approaches based on assembly of prescribed materials from components, illuminates governing principles, and establishes methods for creating precise and

Sidebar: Transformative Manufacturing



Nanomaterial synthesis by assembly is a unique approach for **transformative manufacturing**.

(Top) A 3D framework is formed when DNA lattice frames are coated with silica then templated by either vapor infiltration of the framework, or infiltration by liquid metal salt solutions. The resultant nanolattice after heat treatment is composed of conformal coatings of silica and metal/metal oxide. Scanning TEM cross-sectional analysis of the resulting material.

(Bottom). A wide variety of metal, semiconductor, and insulator compositions can be synthesized by this approach. [Science Advances 10 (2024)] scalable materials. A long-term goal is developing an *inverse design* strategy, wherein synthesis and assembly procedures are defined for achieving targeted structures with desirable functions.

CFN staff research involves creating and applying nano-synthetic and self-assembled nanomaterials, including nanoparticles, DNA, biomolecular complexes, polymers, zeolites, and 2D materials, and integrating them into larger-scale systems. CFN staff and users employ these methods to generate new nanomaterials and devices. For example, CFN staff have used DNA assembly to create materials with unique optical and chemical properties, while block copolymers produce antireflective optical coatings and water-repellent surfaces. Nanoparticle systems have been used to address challenges in catalysis and energy transfer.

The CFN will advance the science of synthesis by assembly by integrating self-assembly methods and nanomaterial synthesis with robotic platforms and autonomous experimentation. AI-guided algorithms will direct material synthesis and fabrication. Automation of synthesis-by-assembly will provide parallelism and reproducibility, enable increasingly complex architectures, provide control of assembly pathways, and allow real-time feedback during processing. AI and machine learning methods for multimodal, *in situ*, and multiscale characterization will provide insights into assembly processes and design principles.

This effort relies on cutting-edge characterization methods such as X-ray scattering, electron microscopy, single-molecule optical detection, spectroscopy, and photon- and electron-based tomography — and will ultimately integrate *in situ* characterization into the synthesis process for real-time structure/property monitoring and feedback.

In the next five years, scientific efforts will be focused on developing of nanomaterial synthesis-by-assembly to achieve architectures with multiple levels of structural and compositional complexity, designed and built to targeted functionalities. Major directions include:

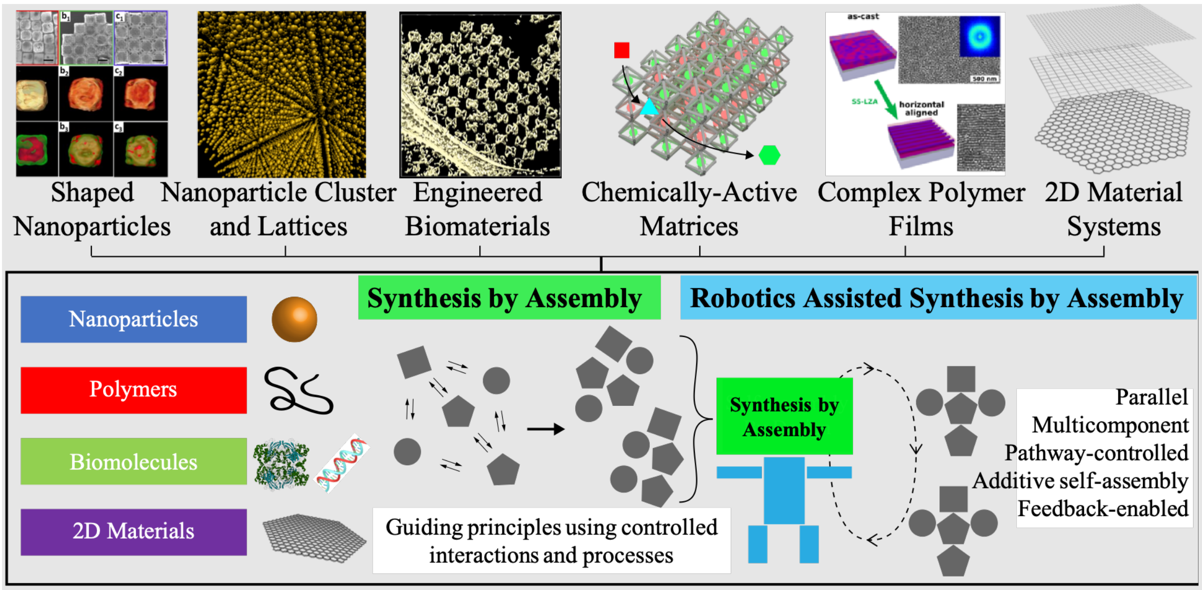


Figure 3. Nanomaterial synthesis-by-assembly is realized through discovery of guiding principles of materials formation and self-assembly by design, and development of effective and broadly applicable material generation methods. Robotic-assisted synthesis-by-assembly platforms will address challenging aspects of AI-guided structure formation for creating nanomaterials with targeted architectures and functions.

- Creating periodic nanoparticle arrays with predefined organization and composition for controlling collective optical, magnetic, and catalytic properties. Nanoparticles with directional bonds will enable the formation of lattices with prescribed symmetry and multiscale internal organizations through synergetic connections of experimental, theoretical, and computational efforts.
- Incorporating functional biomolecular complexes (enzymes, proteins) into nanostructured materials and gaining control over building designed biomaterial systems. Nano-biomaterials can enhance biochemical reactions, promote coupling with inorganic interfaces, and provide new sensing modalities.
- Developing versatile modeling and design tools for realizing rational nanomaterial assembly. Numerical simulations will be used to reveal the interplay of interactions leading to structure formation, understanding and guiding kinetic pathways for high fidelity self-assembly, as well as the structural characteristics at different scales and in response to stimuli.
- Using liquid handling robotics for automated fabrication by assembly, integrating DNA-based assembly platforms with component libraries with rapid on-deck characterization, for programmable nanomaterial design and fabrication.
- Designing assembly pathways for realizing self-assembled nanostructures with control over nanometer to millimeter length scales. By exploiting non-equilibrium behavior and/or integrating top-down and bottom-up methods, it will be possible to manipulate different length scales during self-assembly. For example, photo-thermal stimulation will pattern block copolymer films at the microscale, with molecular-scale self-organization.
- Controlling fabrication of shaped nanomaterials at scales from atomically defined nanoparticles to 3D nanostructures. CFN will continue developing methods for controlling nanoparticle growth mechanisms and will use high-throughput synthesis and multimodal, *in situ* characterization optical and X-ray methods for AI-guided nanoparticle synthesis.
- Developing inorganic templating methods and applying them to complex, self-assembled assembled bio-scaffolds, for control over composition and spatial design of 3D nanomaterials.

To advance these scientific directions, major methods and capabilities will be developed:

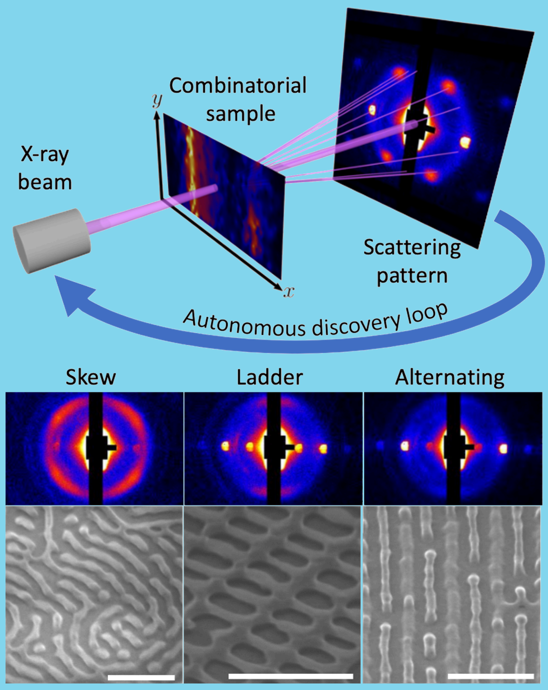
- In situ and time-correlated X-ray scattering analysis for quantitative descriptions of ordered, weakly ordered, and cluster nanoscale organizations and their dynamic behavior at size scales ranging from one to 100s of nanometers, and timescales as short as milliseconds.
- X-ray and electron tomography methods for revealing 3D structural and chemical organization of nanoscale assemblies using photon- and electron-based approaches, with sub-nm spatial resolutions for nano- and mesoscale materials.
- Micro-beam synchrotron light scattering for multiscale and phase mapping of nanostructured multi-component materials on different scales, from molecules to macroscopic dimensions.
- *In situ* nano-mechanical characterization of hard, soft, and hybrid materials for bulk and surfaces, combined with high-resolution imaging by electron microscopy and probing by *in situ* scattering.
- Single-molecule optical methods to probe local optical fields, energy transfer and transduction processes, polarization signatures, and material heterogeneity.

3.2 Theme 2: Accelerated Nanomaterial Discovery

Modern materials are increasingly complex. Formed from a wide range of components, they exhibit structural order at multiple length scales (atomic, molecular, nano, meso, micro, macro) and are synthesized using elaborate processing pathways, frequently in non-equilibrium states. The functional demands on new materials are increasing, designed for performance improvements in next-generation applications (e.g., energy materials, quantum information science, enhanced optical or mechanical properties). Historically, new materials development has followed an iterative process of synthesis, measurement, and modeling. Tightening this discovery loop has potential for radically accelerating the design of new materials and revolutionizing materials science. The CFN is among the leaders in developing next-generation methods for accelerated nanomaterial discovery, including combinatorial sample libraries, robotic synthesis, advanced characterization, machine-learning analytics, and autonomous experimentation platforms that iteratively explore material parameter spaces and uncover fundamental links between synthetic pathways, material structure, and functional properties (**Sidebar**).

As artificial intelligence and machine-learning (AI/ML) methods become more advanced, there is an emerging opportunity to further accelerate scientific discovery. The CFN can play a leading role by demonstrating the potential of a new AI-accelerated paradigm. The CFN will build towards a science exocortex—a swarm of AI agents operating in unison to extend a researcher's cognition and volition (Figure 4). Beyond merely accelerating tasks, the exocortex will be an extension of a person's cognition (memories, thoughts, intents), by frictionlessly surfacing novel trends and ideas, and translating scientific ideas into autonomously executed research directions.

Sidebar: AI/ML in Scientific User Facilities



Autonomous Experimentation. Autonomous X-ray scattering was used to explore the directed assembly of block copolymer thin films. The AI agent was directed to explore the parameter space while searching for novelty. The autonomous search identified three previously unreported polymer morphologies after only six hours of measurement time. [Science Advances **8**, 2 (2023)]

The development of the envisioned exocortex requires frontier methodological research and careful consideration of adapting AI/ML methods to nanoscience research. The proposed architecture for the exocortex reveals a set of research drivers:

- *What are the best ways to connect researchers to automated synthesis & processing platforms*? The CFN has expertise in developing automated research platforms and autonomous experimentation methods and is demonstrating the viability of AI language models for streamlined control of scientific instruments — effectively using AI as an experimental assistant. The CFN will integrate and refine these capabilities to create low-friction interfaces with the researcher, for planning,

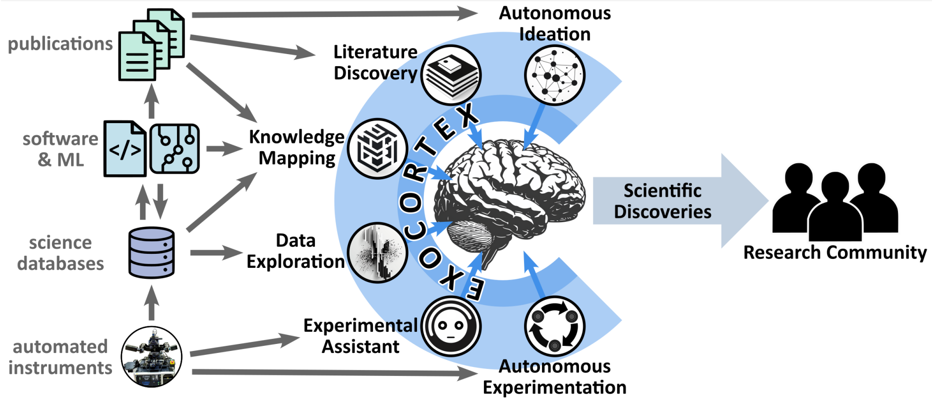


Figure 4. A science exocortex extends the researcher's cognition and volition, by mediating activity through a swarm of AI agents. These agents leverage foundation models (e.g., for language, code, decision-making) to perform tasks such as autonomous experiments, streamline interaction with information (datasets, publications), and enable new ways of AI-human brainstorming. These AI capabilities will be built on top of intrinsically useful components, including: synthesis platforms, open databases, and ML-accelerated analysis code.

launching, monitoring, and modifying complex experiments.

- *How can data streams be integrated into scientific knowledge*? Researchers gain scientific understanding by integrating disparate kinds of information into a coherent model in their minds. CFN will work toward the machine equivalent of such information synthesis, designed to handle the complexity and high dimensionality of modern nanoscience research. For instance, data on a single material from different modalities (images, spectra, simulations, analytic theory) must be mapped into a single, self-consistent predictive model.
- *How can ideation be improved*? Human scientists are uniquely suited to generating new research ideas and new interpretations that advance the state of our understanding. AI is poised to accelerate this process. For instance, AI agents could explore documents to surface relevant information; while other agents could autonomously generate ideas, sorting and triaging them for human exploration. Working with a swarm of agents will facilitate researchers synthesizing and communicating scientific knowledge more effectively.

During the next five years, CFN scientists will conduct fundamental research to research in nanoscience methods, which will combine to enable the envisioned capabilities of the exocortex. Realizing this vision requires advancements and automation of all stages of material discovery: synthesis, especially by implementing combinatorial libraries and real-time synthesis platforms; characterization, including multi-modal *in situ*/*operando* measurements; and understanding, through theory/analytics and use of machine-learning to drive experiments.

- *Autonomous Experimentation*: CFN will investigate improved algorithms for control of experimental platforms, including increasing integration of inputs from theory and simulation. We will leverage large language model (LLM) technology to build experimental assistants, which will provide streamlined control of complex instruments, including experiment execution, autonomous loops, and data analysis. We will deploy proven methods across a broad range of nanoscience instruments.
- *Synthesis Platforms*: The CFN has invested significantly in developing materials synthesis platforms, including the Quantum Material Press, a photo-thermal annealer for thin film non-equilibrium physics, a spray deposition tool for adaptive synthesis of soft materials, a flow-reactor for nanoparticle synthesis, and a robotic liquid handler to automate voxel-assembly

strategies of complex architectures using DNA self-assembly. The CFN will continue developing these and other platforms, targeting their use in accelerating the research loop.

- *Science Agents*: CFN will concretely design, test, and deploy infrastructure for advanced science workflows. For instance, we will implement LLM capabilities to investigate whether AI agents can productively engage in autonomous ideation. We will transition CFN experimental datasets into robust database environments and build ML workflows that operate on these databases. We will ML data exploration tools, to provide nanoscience researchers with new ways to identify trends in their data.

3.3 Theme 3: Nanomaterials in *Operando* Conditions

Characterizing nanomaterials during operation in their native environments is vitally important to modern materials science. External stimuli, including pressure, temperature, light, and voltage, lead to dynamic material changes, which may only be observable under functional conditions. Discovery of structure-function relationships hinges on *in situ* material investigations. For example, synthesis of new catalysts hinges on identifying active phases and reaction mechanisms, *as they emerge at the elevated pressures, environments (liquid or gas), and operating temperatures*. Environmental scanning transmission electron microscopy (E-STEM) and local-area electron energy loss spectroscopy (EELS), scanning probe microscopy (SPM), low energy electron microscopy/X-ray photoemission microscopy (LEEM/XPEEM), vibrational (IR and Raman) spectroscopy, and ambient-pressure photoemission spectroscopy (AP-PES) comprise an experimental toolset capable of *operando* nanomaterial interrogation. Atomic scale theory links key structural motifs to complex spectra and observed characteristics.

The CFN has assembled a comprehensive suite of tools for understanding materials as diverse as catalysts, quantum materials, and battery electrodes. *In situ* and *operando* implementations of these core techniques are a frontier area of research, as is their integration for multimodal studies (Figure 5). Time-resolved perturbations by modulation excitation spectroscopy (MES) can provide additional kinetic information (**Sidebar**). The CFN is incorporating time-resolved techniques into X-ray & vibrational spectroscopy and electron microscopy, and leveraging ML driven methods to aid in the interpretation of the resulting complex spectrokinetic datasets. In the next five years, the CFN will further advance capabilities for *in situ* and *operando* measurements and integrate them with others being developed at NSLS-II. For example, we will substantively expand in situ environmental electron microscopy capabilities by installing a unique monochromated, aberration-corrected UHV E-STEM capable of spanning nine orders of magnitude in pressure, and a second

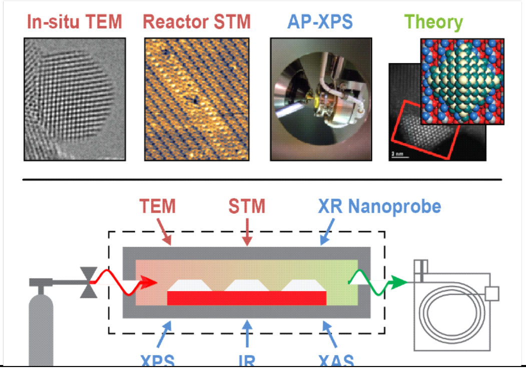


Figure 5. Nanomaterials in *Operando* Conditions. The CFN portfolio of *in situ* and *operando* techniques using electrons, ultrafast photons, and X-ray radiation, coupled with theory, creates a unique setting for studying the link between structure and function of nanomaterials. A key element of this approach is correlating multimodal imaging and spectroscopy with real-time reactivity measurements. This can be done using portable high-pressure reaction cells in which the same materials are interrogated in *operando* by electron probes at the CFN and complementary photon probes at NSLS-II or using a vacuum suitcase for transferring samples among ambient pressure systems and reactors.

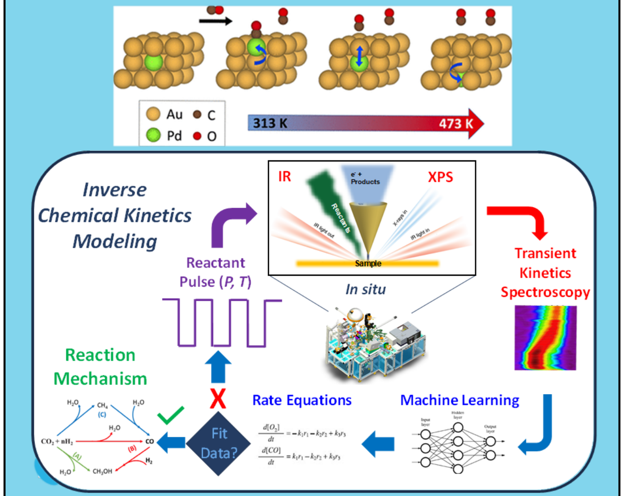
STEM equipped with a secondary electron detector for simultaneous surface and through-sample imaging. AI/ML methodologies will be developed to rapidly distill information from the massive amounts of imaging, diffraction, and spectroscopy data generated by these instruments.

CFN users and staff are interested in catalysts for greenhouse gas-to-fuels and biomass conversion, with metals incorporated inside or dispersed on nanoporous materials such as zeolites and metal organic frameworks. Chemistry in nanoconfined spaces can affect the formation of active centers and reaction pathways, and can change the required reaction conditions. Copper-based catalysts, for example, show promise for hydrogenation of CO_2 to methanol and direct conversion of methane into alcohols. Stabilization of active Cu ensembles in nanoporous materials with high local effective pressures can facilitate their detailed study under *operando* conditions.

In situ characterization is important for understanding photocatalytic water splitting. Photocatalysis requires separation of photoexcited charge carriers on ultrafast timescales, to avoid recombination losses. Ultrafast optical spectroscopy is uniquely suited to quantifying recombination losses and understanding how they can be suppressed through nanoscale material and interface design. Catalytic steps occur on longer time scales, and changes in the local structure of active centers can be understood using spectrokinetic XAS, AP-PES, and IR measurements under *operando* conditions.

Energy storage is a third area where probing materials in complex environments can yield new insights. Creating electrochemical batteries with both high storage capacity and high cyclability requires understanding electrochemical processes at electrode/electrolyte interfaces, including structural and phase changes, electron/ion insertion mechanisms, and the dynamical evolution of the interface structure. CFN users studying Li-ion (and other alkali-ion) batteries are interested in resolving the reaction pathways and unlocking the potential of novel materials such as disordered layered oxides as battery electrodes. Combining synchrotron-based techniques with *in situ* electron microscopy using specialized electrochemical or biasing holders provides critical insights into these processes.

Sidebar: Clean Energy



Dynamic single atom catalysts. Dynamic restructuring of alloyed catalysts plays a crucial role in their activity and selectivity. Unraveling the kinetic parameters of elemental processes can help guide their development for **clean energy** applications.

(Top) CFN researchers have implemented time-resolved temperature-programmed IR spectroscopy for *in situ* studies of dilute components in nanomaterials and single atoms.

Working with the Integrated Mesoscale Architectures for Sustainable Catalysis EFRC, CFn scientists followed the stabilization of surface palladium single atom catalysts by the presence of carbon monoxide reactants [J. Am. Chem. Soc. **144**, 15132 (2022)].

(Bottom) Current work includes integrating ML-aided real time analysis of reaction mechanisms with experiments [J. Chem. Phys. **157**, 164801 (2022)], for actively controlling catalytic process selectivity using external stimuli.

In the next five years, CFN scientists and users will make use of this wealth of capabilities and expertise to understand nanomaterials under *operando* conditions, working on:

- Elucidating catalytic reactions through integrated measurements by Reactor STM, AP-PES, IR, Raman and UHV E(S)TEM, each operating at elevated local pressure and temperature;
- Optimizing separation of photogenerated charged carriers at nanostructured hybrid organometallic/oxide interfaces of photocatalysts using *in situ* ultrafast optical spectroscopy and light-modulation excitation spectroscopy and operando X-ray spectroscopy at both CFN and NSLS-II;
- Investigating reaction pathways in the electrode structure of energy storage systems using (S)TEM-based methods with high spatial, spectral and temporal resolution.

CFN scientists will advance *in situ* and *operando* instrumentation by:

- Commissioning a unique UHV environmental, monochromated, aberration-corrected scanning transmission electron microscope designed for high-resolution studies of structural and chemical evolution of nanomaterials in different gas environments;
- Extending CFN AP-PES capabilities by commissioning a new instrument with a multicolor tender X-ray source. Combining this instrument with new liquid cells will enable studies of liquid/solid interfaces, including during synthesis and electrochemical processes;
- Developing computational methods, such as improved first-principles approaches and AI/machine learning, to link atomistic structures to spectroscopic, imaging, and/or diffraction signatures obtained from simulated materials or structures on databases. We will also develop methods to unravel the controlled growth of thin films and catalytic reaction pathways from data obtained under synthesis or reaction conditions.

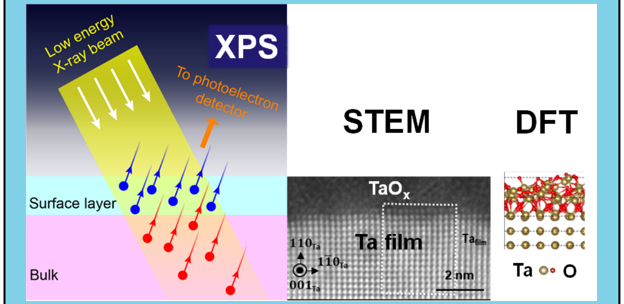
3.4 Crosscut 1: Multimodal Nanoscience

A crosscutting strength of CFN is supporting integrated, complementary capabilities for multimodal nanomaterial investigations. The high levels of complexity in modern materials demand characterizations of multiple properties (e.g., structure, morphology, composition) to gain a full atomic and molecular understanding of fundamental processes (**Sidebar**).

Traditionally, these types of characterizations are performed using different instruments and samples, creating uncertainty and variability. For example, unravelling the role of heterogeneity in size, structure, and composition in alloy catalysts requires both characterization of ensemble average chemical properties using X-ray and vibrational spectroscopies, and local measurements of individual structures and elemental distributions using high-resolution microscopy.

The CFN continues to focus on creating compatible experimental platforms that integrate material synthesis with a suite of

Sidebar: Quantum Information Science



Tantalum is a promising material for superconducting qubits and has enabled record-long coherence times. Understanding the underlying reasons for qubit decoherence can yield material design pathways to ever better qubit performance.

In collaboration with the Co-design Center for Quantum Advantage (C2QA), CFN has led multimodal studies correlating tantalum surface oxidation states with coherence losses. A variable energy X-ray photoelectron spectroscopy methodology was key to revealing the depth profile of tantalum oxidation [*Advanced Science* 2023, 2300921]. Integrating X-ray measurements with electron microscopy and an atomistic model gives a more complete picture of complex surface oxide formation [*ACS Nano* 2024, 18, 1126].

complementary advanced characterization. These platforms provide the nimbleness required to rapidly respond to new materials developments and science initiatives. Coupled with development of experimental platforms, CFN will advance accompanying methods in data analytics to extract and interpret information derived from multidimensional datasets.

In support of the crosscutting CFN effort to provide an expanding platform for multimodal material investigations, during the next five years we will:

- Design, acquire, and assemble a suite of portable gas or liquid reactor cells, enabling studies of the same catalyst or battery material under identical environmental conditions by S/TEM, AP-PES, and X-ray spectroscopies at NSLS-II. These cells will measure gas pressure, reactant/product composition, temperature, and pH. We will standardize a universal sample holder for sample transfer in vacuum/inert gas among CFN and NSLS-II capabilities.
- Commission an aberration-corrected UHV ESTEM that spans nine orders of pressure, with gas handling & mixing and integrated UHV capabilities for sample preparation and characterization.
- Design. acquire, and assemble hardware and software for enhancing the temporal, spatial, and spectral resolution of electron microscopy, to bridge resolution gaps with surface science and synchrotron techniques and promote more seamless multi-modal characterization.
- Develop and use AI/ML methods, coupled with simulations, for increasingly rapid analysis of imaging, diffraction, and spectroscopy data acquired by in situ electron microscopes — to extract useful information such as trigger events (e.g., nucleation, phase transformations), 4D-STEM, and EELS.
- Commission a unique facility for multimodal, low-temperature characterization of key properties of stacked, 2D quantum material heterostructures. The facility (QM-IMCP) will comprise low temperature synchrotron spectro-microscopy, ultrafast pump-probe magneto-optical microscopy, and multimodal SPM with quantum sensors. QM-IMCP will be fully integrated with the Quantum Material Press for combined automated synthesis and multimodal characterization in a single workflow.
- In partnership with the BNL-led Co-design Center for Quantum Advantage (C2QA), we will design and build a first-of-its-kind milli-Kelvin Scanning Probe Microscope with multimodal probes, including a high-Q stripline resonator, a superconducting quantum interference device (SQUID), a single electron transistor, and a capacitance sensor, to fully map local energy dissipation, electron spin, and dielectric properties of quantum materials and devices.

3.5 Crosscut 2: Artificial Intelligence and Machine Learning for Nanoscience

Artificial intelligence (AI) and machine learning (ML) are tools that hold promise for revolutionizing the ways that nanoscience research is conducted. Advancing this exciting, transformative opportunity is a guiding vision that crosscuts many CFN research and facility plans. The CFN AI/ML strategy is to develop adaptable, accessible, and robust tools for data processing, instrument operation, and generation of reliable simulation data (Figure 6). Through staff expertise and hardware facilities, CFN will foster AI/ML adaptation and stake a position as a facility that aligns user scientific needs with appropriate tools.

In the next five years, CFN scientists will advance three primary AI/ML-related objectives:

Real-time interpretation of X-ray, microscopy, and imaging data. CFN is working toward a vision in which future AI/ML tools providing real-time insights during an experiment, e.g., spectra-structure mapping of multiphase nanomaterials during X-ray characterization. By liberating scientists of domain-specific routine tasks, CFN staff and users will redirect their attention to more substantial challenges and critical aspects of scientific discovery.

Autonomous operation of advanced instrumentation. Advanced CFN experimental capabilities (e.g., high-resolution atomic force microscopy) are most often extremely complex to operate, requiring the expertise and dedicated time of staff members. Ultimately, this limits their broadest availability to the user community. CFN will work to create user-friendly AI/ML tools to simplify instrument operation, through automation and eventually autonomizing experiments.

Accelerating physics-based modeling. While known physiochemical principles govern many aspects of nanomaterial function and reactivity, there is insufficient data from physical models to feed into data-centric approaches. ML-acceleration of materials modeling has been shown to have impressive speed-up. CFN will extending these methods to calculations of functional properties, connecting large-scale complex systems to the AI/ML learning process.

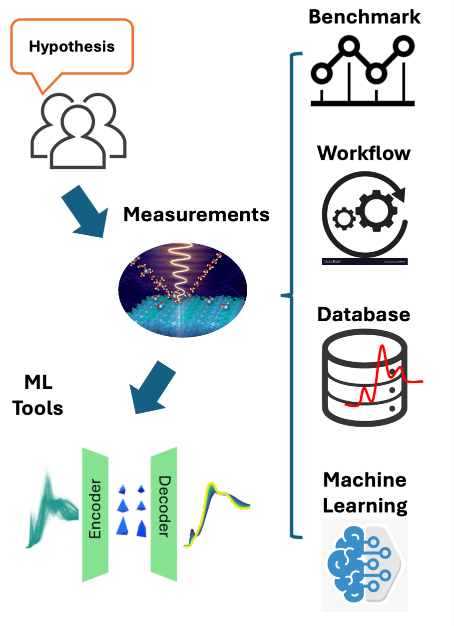


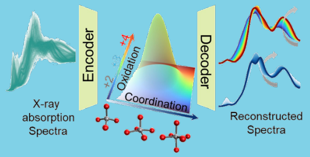
Figure 6: The hierarchy of AI/ML tools and development includes benchmarking to quantify key approximations and to validate theory against experiment, workflows for ensuring consistency, reproducibility and interoperability of in datasets, diversified database construction and management tools, and AI/ML models to solve forward/inverse problems and produce interpretable models. These technical developments will advance scientific discovery and the DOE user community, making BNL a destination for researchers to carry out all stages of nanomaterials discovery.

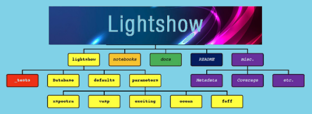
Ongoing and targeted developments include:

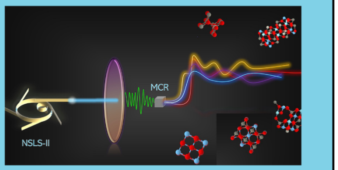
- A suite of tools that develop data driven XAS analysis from curation, computational modeling, and data analysis (**Sidebar**).
- Development of ML algorithms to interpret big data streams from ultra-fast direct electron detectors to advance CFN electron microscopes capability. Software development and data management will be done in partnership with other national labs with CFN leading data analysis tools for automated image analysis and ML models to interpret EELS data.
- Improved ML methodologies for identifying the number of layers in 2D nanomaterials prepared using exfoliation with contrast in optical images.
- Utilizing generative models to address inverse kinetics problems enhances predictive capabilities for reaction mechanisms. Models that offer interpretability and allow incorporation of limited data will leverage CFN developments in spectrokinetics measurements. The capability to model the time dynamics of heterogeneous reactions informs processes relevant to clean energy.

- Enabling AI to recognize common patterns in scanned probe microscopy experiments through ML training, transferring routine tasks from the operator to the instrument. Adding ML decision-making tools and developing models to identify the chemical structures of imaged molecules.
- Launch CFN FrontPage for tools, agents, and workflows. CFN can bridge staff expertise and the fast-evolving nature of AI/ML tool development to magnify productivity of users. An accessible interface based on inputs about scientific or data processing goals can facilitate connecting users to appropriate capabilities and resources.

Sidebar: AI/ML in Nanoscience User Facilities







Advances in data-driven XAS have been achieved through a hierarchal approach incorporating benchmarking [Phys. Rev. Mater. 8, 013801 (2024)], workflow development [J Open Source Softw. 8, 5182 (2023)], database construction, and ML model development [Phys. Rev. Mater 7, 053802 (2023)].

Cross-disciplinary CFN collaborations with NSLS-II and the BNL Computational Science Initiative enables new opportunities in high-throughput materials discoveries, creating many opportunities to address future materials needs.

A new generative AI model, RankAAE, enables discovery of relationships between X-ray spectra and material structure. The Lightshow workflow for computational XAS is a user-friendly tool for improveing synthetic data consistency and reproducibility, essential to data-driven applications.

4. PILLARS

Achieving the Objectives of this Strategic Plan requires an expert and diverse staff, an engaged and diverse user community, and a set of strategic research partnerships. World-leading research by staff and users must be conducted safely and supported by both excellent operations and state-of-the-art facilities. Implementing this Plan requires strengthening these essential pillars, as detailed here.

4.1 Safety and Operational Excellence

Excellence in operations and a strong safety culture are central to CFN success. The CFN emphasizes the importance of communication and training among the staff and users with diverse backgrounds and experiences as the best approach to achieving safety compliance. A robust operational and administrative infrastructure supports the research experience from concept to project completion. Safety is fully integrated into all aspects of the work. Regularly reviewed and updated course modules and on-the-job training are essential for safe and productive research. Prior to independent use of CFN facilities, every new user is trained in general and work specific operations and safety procedures. New users are paired with an expert mentor for guidance on operations, hazard identification, and response. Focus areas for operations and safety include:

- More tightly integrating safety standards and guidelines, operational procedures, and administrative support for planning and executing research;
- Implementing a project planning process to instrument acquisition, installation, commissioning, and operations that reduces and controls hazards;
- Continuously improving a team-oriented work planning and control process to enhance efficiency and safety in service and maintenance of CFN instruments;
- Developing a facility master space plan to guide new instrument installations and workspace allocation; Acquiring lab space in other BNL complex buildings, as needed; renovating

current lab space for new equipment; decommissioning old equipment, and upgrading existing equipment to modernize capabilities.

- Improving the user proposal submission, review, and allocation process for better usability and coordination with other BNL facilities;
- Integrating web-based modules designed for efficient user and staff training into a robust system to ensure that requirements are met prior to granting access to CFN facilities;
- Improving records management and data storage/access for operations and scientific activities;
- Implementing a "cradle to grave" materials safety concept, placing equally high emphasis on nanomaterials and chemical safety from project inception, through project execution, to final material disposal.

4.2 Expert and Diverse Staff

Recruiting, developing, and retaining a diverse group of the highest-quality scientific, technical, and administrative staff is central to fulfilling the CFN mission. Central to this is sustaining a participatory culture for a positive work environment that promotes collaboration and equity. This starts with frequent, open discussions about CFN values and mission. The CFN strives to maintain an environment where all staff feel respected as team members whose professional skills are essential to advancing the CFN mission. Key components of the CFN strategy include:

- Recruiting, developing, and retaining a diverse workforce of the most talented professionals at all levels;
- Creating a positive, inclusive work environment by promoting collaboration and fairness;
- Practicing transparent, meaningful two-way communication;
- Nurturing professional development through thoughtful mentoring for staff members at all career stages, and toward appropriately balanced science and user support efforts;
- Seeking internal and external recognitions for staff professional achievements;
- Maintaining vibrant postdoctoral researcher and graduate student programs (in coordination with the BNL Association of Students and Postdocs), which increase the scope of CFN research and provide opportunities for staff to develop supervisory and mentoring skills;
- Fostering an environment in which scientific staff engaged with external research opportunities, especially those connected to national science initiatives. Examples include: BNL Laboratory Directed Research and Development program, DOE Early Career Awards, DOE Energy Frontier Research Centers, Small Business Innovation Research Programs, and partnering with users in other DOE initiatives.

4.3 Engaged and Diverse User Community

To fulfill its mission of serving a satisfied and productive user community, the CFN continuously engages past and current users and actively seeks communities of new users. Users are integral to the CFN culture and planning, well beyond facility usage and staff collaborations. The CFN strives to identify and eliminate barriers hindering user research, to support the broadest community of users more effectively, through activities that include:

- Engaging early career scientists to maintain the vibrancy of the user program, deliver frontier research that encompasses the most forward-looking knowledge, and develop the next generation of nanoscience researchers and educators;

- Fostering transparency and cooperation through an engaged Users' Executive Committee (UEC). The CFN UEC provides an organized framework for communicating user needs to CFN and BNL management. Together, NSLS-II and CFN UECs organize the annual Users' Meeting, with support from CFN staff. The CFN regularly engages the UEC for input on how to best support a diverse user community.
- Enhancing the User Experience. The CFN strives to optimize the user experience, from proposal submission and review/allocation, instrument scheduling, data collection, and dissemination of research findings.
- Advancing Remote@CFN. The CFN continues to expand its ability to support users who are not physically present at the facility. Remote@CFN has facilitated remote engagement of users with CFN staff, remote operation of instruments during experiments, and off-site access to experimental data and CFN-supported analytics software.
- Promoting User Science. The CFN promotes user science through BNL newsroom stories, social media, the *iCFN* newsletter, and research highlights.
- Engaging in Strategic Partnerships. CFN staff engage with user teams when there is a clear alignment of scientific interests, *e.g.*, Energy Research Frontier Centers and Small Business Innovation Research (SBIR) projects.
- Reaching New and Diverse Users. CFN is working to expand the diversity of users by deploying staff as ambassadors at scientific meetings and conferences. An element of the strategy is reducing barriers for underrepresented groups to access CFN.
- Providing Technical Workshops. Instrument/technique training and user development workshops are excellent ways of linking CFN staff and experienced users with targeted potential users over topics of shared interest. These events and complementary tutorials serve as effective outreach to expand the user community and strengthen engagement.

4.4 State-of-the-art Facilities

The CFN facility is envisioned with the entire process of materials research in mind, with users accessing an integrated set of tools for a complete research experience under one roof. To that end, we operate advanced instrumentation in materials synthesis, nanofabrication, electron and photon probes, and computational resources with software tools for theory, simulation, and data analytics.

The CFN portfolio is strategically refreshed to provide cutting-edge facilities attractive to high-impact users. We balance upgrading existing major capabilities with acquiring key new instruments. This Plan envisions investments driven by the needs and trends in major materials research initiatives. For example, in the next five years:

Materials Synthesis and Nanofabrication

CFN will make significant investments in the nanofabrication facility to enable more sophisticated research and provide a more user-friendly experience:

- *Electron-beam Lithography*: State-of-the-art, 200kV electron-beam lithography system optimized to support a broad range of research. Improved writing speeds of >100MHz will facilitate high throughput exposures and large area patterning (cm^2 or larger) critical for many applications including synchrotron experiments and combinatorial studies.
- *Direct Write Laser Lithography*: Maskless photolithography via a rastered, focused UV laser beam provides great flexibility and patterning arbitrary designs with micron-scale critical dimensions.

- *Combinatorial Thin Film Deposition*: State-of-the-art physical vapor deposition tool will expand the range and complexity of materials synthesis, by providing co-sputtering, reactive sputtering, and compositional gradient films.
- *EUV Interference Lithography*: Synchrotron instrument for interference lithography at the extreme ultraviolet (EUV) wavelength (13.5 nm) used in modern lithography tools. This instrument will enable research on materials and methods for "Angstrom-era" nanofabrication, critically needed for advancement in the semiconductor industry.

Liquid-handling robot upgrade: The CFN has established a liquid-handling robotic platform for automated synthesis-by-assembly of multicomponent systems including nanoparticle-based materials, DNA structures, and designed biomaterials. An upgrade to this system will incorporate in-line characterization and AI/ML guided feedback control.

Electron and Photon Probes

QM-IMCP: The CFN Quantum Materials Integrated Multimodal Characterization and Processing platform (QM-IMCP) will offer precise assembly, processing, and multimodal characterization of heterostructure quantum materials. Providing a unique set of complementary cryo-probes, QM-IMCP will facilitate transfer of materials and analysis of the same feature across the suite:

- Atomic layer etching of 2D and quasi-2D materials, providing atomically precise control over material thickness.
- Cryogenic upgrade to the aberration-corrected low-energy electron microscope / photoemission electron microscope (AC-LEEM/XPEEM) operated at NSLS-II will enable cryogenic operation.
- Multimodal cryogenic scanning microscope with integrated quantum sensors will provide a testbed for quantum methods of sub-nm electrometry, magnetometry & spectroscopy.
- A cryogenic, ultrafast pump-probe magneto-optical microscope, realized by coupling a new cryostat/magnet assembly with an existing ultrafast pump-probe microscope.

MilliKelvin Multiprobe: This unique in the world scanning probe microscope will perform multimodal ultrahigh-sensitivity measurements at millikelvin temperatures, correlating spatial changes in magnetic, electronic, and dielectric properties. Given the large size of devices like superconducting qubits, probes will be engineered with a sensor area of several square microns.

Low-Voltage scanning transmission electron microscope STEM: A state-of-art STEM for high-resolution studies of electron-beam sensitive materials will have an ultra-bright, cold field-emission gun with aberration correction and monochromator for atomic resolution imaging at low voltage and low electron dose, with state-of-the-art <5 meV electron energy loss spectroscopy (EELS) resolution.

Ultrafast Camera for ETEM: In collaboration with Berkeley Lab and the BNL Computational Sciences Initiative, a unique, ultrafast direct electron detector attached to the Titan aberration corrected ETEM will enable image capture at 87,000 frames per second — a first-of-its-kind capability for atomic-scale, operando studies of material dynamics on microsecond timescales.

E-STEM: An aberration-corrected environmental scanning transmission electron microscope (E-STEM) that is probe-corrected monochromatic, UHV microscope with atomic spatial resolution and state-of-the-art ~5 meV electron energy loss spectroscopy resolution. This E-STEM allows gaseous environments at the sample from UHV to 10 Torr for *in situ*/operando experiments.

High-resolution TEM/STEM: A 200kV transmission /scanning transmission electron microscope (TEM/STEM) for high-resolution structural and analytical characterizations. This TEM/STEM will be equipped with an energy-dispersive X-ray spectrometer for elemental analysis and a camera for a large field of view.

Synchrotron X-ray Scattering: The CFN will continue to invest in the Complex Materials Scattering (CMS) and Soft Matter Interfaces (SMI) beamlines, partner X-ray scattering endstations at NSLS-II. High-throughput and autonomous experimentation will be further developed through advanced software tools and real-time materials processing platforms.

HAXPES: A new instrument featuring a multicolor tender X-ray source will enhance CFN lab-based AP-PES capabilities. The variable X-ray energy will provide three sample probing depths, broadening the range of sample environments for AP-PES analysis. The tender X-ray source enables investigations of gas/solid interfaces at 1 atm.

X-ray Tomography: This state-of-the-art x-ray tomography will be capable of x-ray imaging in 2D and 3D with sub-50 nm spatial resolution and with fields-of-view as large as several tens of microns. The instrument will have cells for *in situ* imaging in liquid and gas environments.

Laser Upgrade for PEEM: An upgrade to the CFN XPEEEM/LEEM system with a supercontinuum IR-UV laser for pumping electrons from valence to conduction bands while simultaneously probing the electronic structure with XPEEM/LEEM.

Lab SAXS Upgrade: A high intensity metal jet x-ray source will provide substantially more brightness, and robotic sample handling will enable experiment automation.

Computational Resources

HPC upgrades: Innovative software and data management, including use of machine-learning tools, and development & applications of physical theory, will be supported by regular CFN investments in new high-performance and high-throughput computing capabilities, data storage, and communications in cooperation with the BNL Scientific Data and Computational Center.

4.5 Partnerships

Building upon a culture of collaboration and innovation, the CFN will establish and strengthen strategic partnerships to best apply CFN research expertise and capabilities in support of major DOE initiatives, e.g., the BNL-led, Office of Science QIS Center: Co-Design Center for Quantum Advantage (C^2QA) and Energy Frontier Research Centers in catalysis and energy storage. Intellectual property and technology transfer are other ways to connect with industry researchers, such as through the DOE SBIR program and Technology Commercialization Fund. Partner users provide investments of expertise and equipment that help CFN grow in new directions.

The CFN operates within the larger BNL environment, which has offices overseeing institutional Diversity, Equity & Inclusion (DE&I) initiatives. CFN strongly partners with these offices to augment our efforts with additional resources and expertise. Examples of DOE programs that CFN makes use of are: SULI (for undergraduates), SCGSR (for graduate students), and the Visiting Faculty Program (for faculty and students). The CFN is deeply involved in BNL programs fostering diversity (e.g., Interdisciplinary Consortium for Research and Educational Access in Science and Engineering (INCREASE), with which CFN partners to host workshops for potential users from HBCUs, Tribal Colleges, & HSIs) and mentors GEM Fellows working with CFN staff.

The CFN partnership with NSLS-II

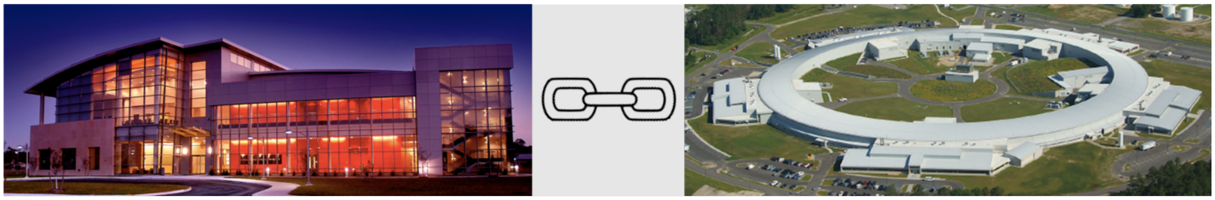


Figure 6. A strong partnership with NSLS-II is a key element of the Strategic Plan. Three illustrative areas are:

Theme 1: Nanomaterial Synthesis by Assembly

The CFN is a world-leader in DNA programmable self-assembly of heterogeneous nanomaterial lattices. CFN is developing methods using the advanced beamlines at NSLS-II to study how self-assembly can be used to organize targeted nanocomponents, especially optically and chemically-active species, into well-defined functional lattices.

Theme 2: Accelerated Nanomaterial Discovery

CFN is developing autonomous experimentation methods. Machine-learning methods have been created to automatically analyze X-ray scattering and spectroscopy data. Algorithms for autonomous experiment control have been developed in collaboration with the DOE CAMERA project. In partnership with NSLS-II, these concepts have been implemented at multiple beamlines for autonomous exploration of materials parameter spaces.

Theme 3: Nanomaterials in *Operando* Conditions

CFN and NSLS-II staff operate a low energy electron/X-ray photo-electron emission microscope (LEEM/XPEEM) endstation, and have implemented cells and data analytics for hard X-ray absorption spectroscopy (XAS) at NSLS-II. Combining information from *operando* experiments at NSLS-II endstations and the CFN environmental transmission electron microscope (E-TEM), critical information from dynamic processes in catalysts can be interrogated.

The CFN will continue to deepen the relationship with NSLS-II through investments in X-ray nanoscience instrumentation, joint projects, and streamlined access mechanisms (Figure 7). This relationship between facilities strongly benefits users and staff. Some examples include:

- Development and management of new X-ray nanoscience instruments and Partner User Agreements with NSLS-II to support users at four endstations. These ventures represent leading capabilities in X-ray scattering, photoelectron spectromicroscopy, and X-ray tomography. CFN contributes essential equipment and staff & helps users access unique experimental capabilities.
- CFN capabilities and expertise are applied to developing new capabilities at NSLS-II. For example, CFN nanofabrication is used to create high-performance X-ray optics, beam sensors, and reference samples for method development at beamlines.
- The CFN will continue to establish joint projects with NSLS-II staff and users. For example, CFN is making use the complementary properties of X-rays and electrons to image the same catalyst under realistic operating conditions, to interrogate working photo-electrochemical systems, and for imaging and spectroscopy of soft and hybrid hierarchical systems.
- CFN and NSLS-II are collaborating to develop and implement data analysis & machine learning software for large data sets from synchrotron and electron microscopy experiments.

5. METRICS & RESOURCES

5.1 Metrics

The ultimate measure of success for this Plan is the extent to which the CFN supports a community of users and staff renowned for nanoscience breakthroughs and societal impact. Each year, CFN reports progress to DOE and receives feedback through the Performance Evaluation and

Measurement Plan (PEMP). Every three years, the DOE evaluates CFN facility operations, with external reviewers assessing the impact of internal research and user science, user satisfaction, and efficiency of facility operations. Annually, the CFN management team, supported by the external CFN Science Advisory Committee (SAC), assesses progress in executing this Plan.

Internally, we measure progress in mission-critical areas using trackable metrics:

- Operating a world-class nanoscience user facility
    - Have the scientific facilities performed optimally and been available to staff & users?
    - Have the scientific facilities been used by users and staff, and contributed to publications?
    - Have the scientific instruments and the entire CFN facility been maintained on a regular schedule, to keep them in optimal condition?
    - Has the CFN continued to evaluate and improve internal processes for more efficient operations and better tracking of performance?
- Developing unique capabilities for the user community
    - Have new capabilities been fully available to CFN users, and have users used them?
    - Have new capabilities led to impactful studies not previously possible?
    - How satisfied are users with the facilities and support provided by CFN staff?
- Fostering the success of world-class scientific staff
    - Has CFN-led research resulted in scientific breakthroughs, published in top journals and widely cited?
    - Has execution of the research plan generated new intellectual property?
    - Are CFN staff members in leadership positions within their respective fields, recognized for their accomplishments by the external technical community?
- Being an essential resource for collaborative research
    - Is the CFN engaged in multidisciplinary research partnerships involving academia, other national laboratories, and industry?
    - Is the CFN considered an essential resource in large-scale efforts in scientific areas of national interest?
    - Are CFN scientists key members of collaborative teams in their areas of expertise?

5.2 Resources

Guided by user feedback, input from the UEC, and advice from the SAC, the CFN allocates resources (equipment, staff, operating funds) to support each facility and ensure that high-impact research is carried out in each thematic area. CFN operations are funded by a block grant from the DOE Office of Science. From this budget, the CFN targets investing at least 10 percent each year in new scientific equipment. Projecting realistic future budget increases based on past history, the CFN anticipates being able to carry out this Plan over the five-year period described here.

Fullest impact and utilization of the capabilities developed in the scope of this Plan will require the CFN to add scientific staff in strategic areas. Additional operations funding, beyond budget projections, will further enhance unique CFN capabilities.

If resources are more limited in the future, the CFN will adjust the scope of this Plan accordingly and adopt a conservative approach toward hiring additional staff. In such a scenario, the CFN will establish priorities based on progress among the scientific themes, growth of high-impact facility usage, and input from the SAC and the user community, to ensure that the CFN fulfills its core mission and continues to thrive.