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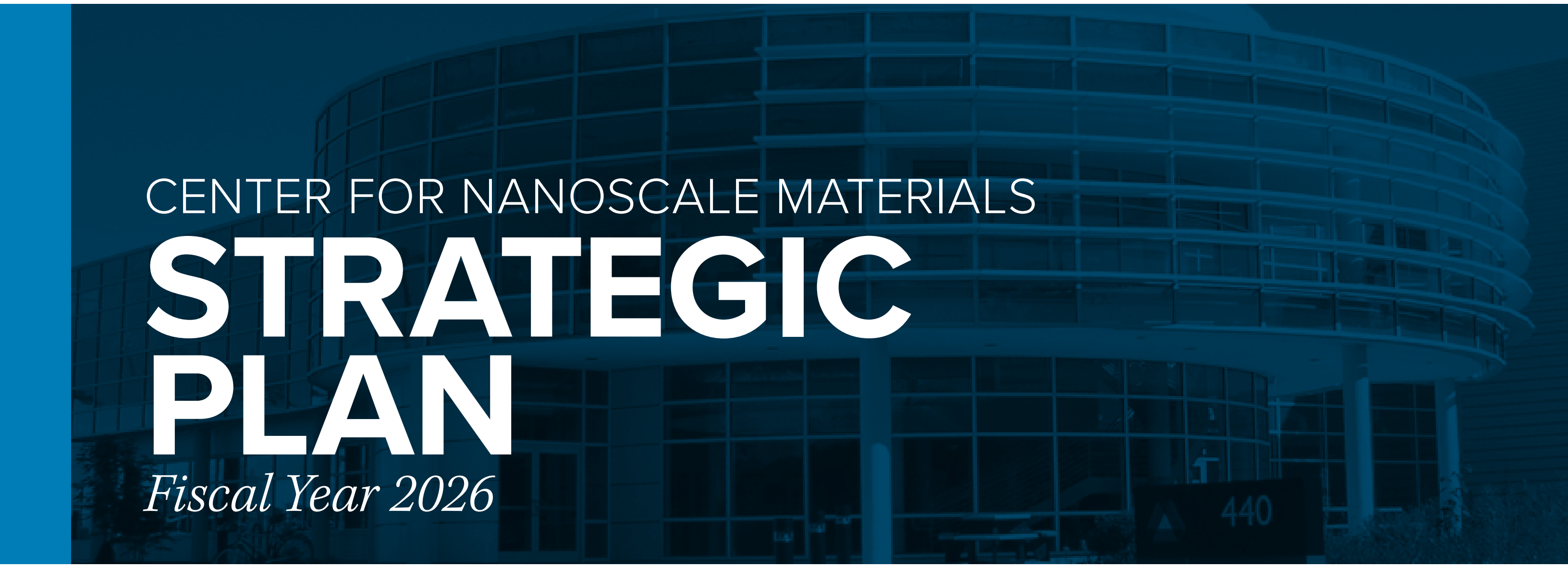
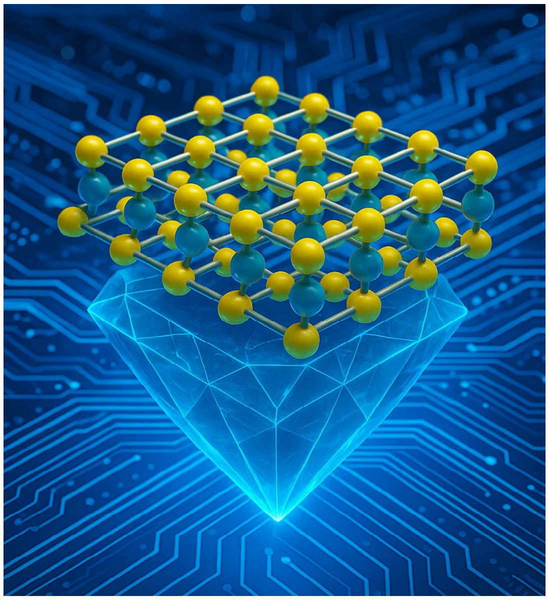
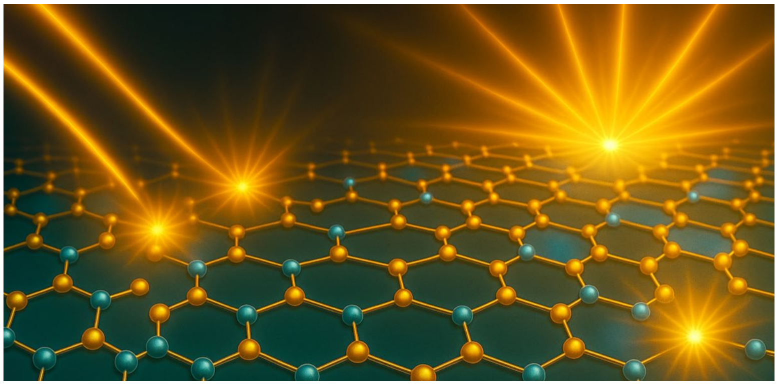


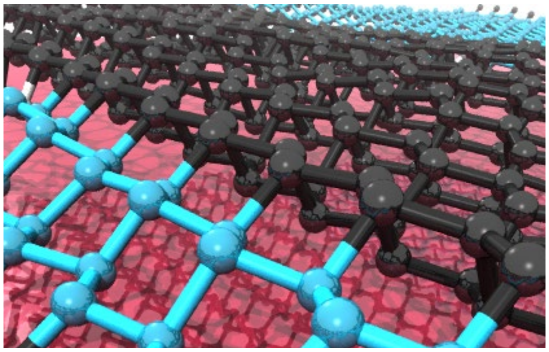
CENTER FOR NANOSCALE MATERIALS

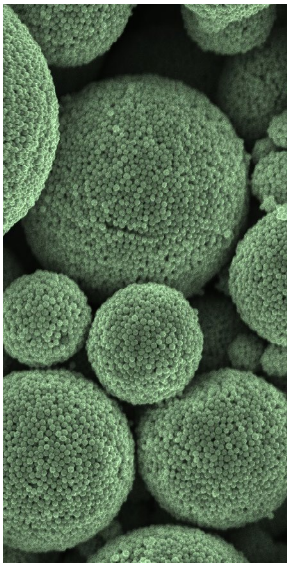
STRATEGIC PLAN

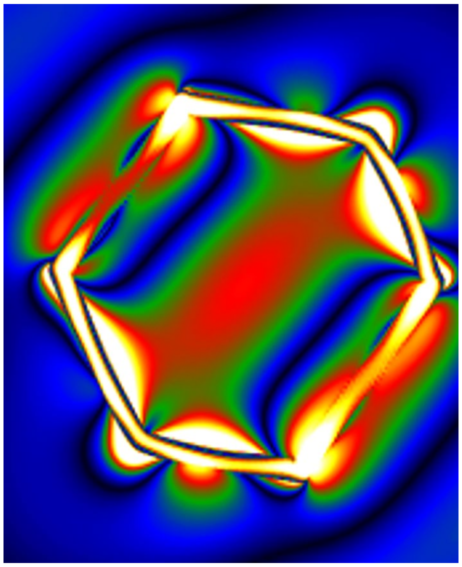
Fiscal Year 2026











U.S. DEPARTMENT of ENERGY

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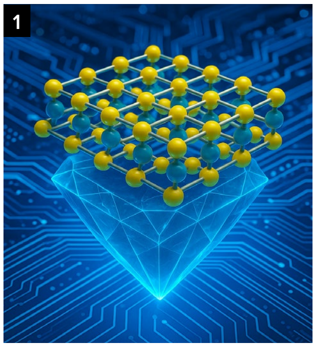
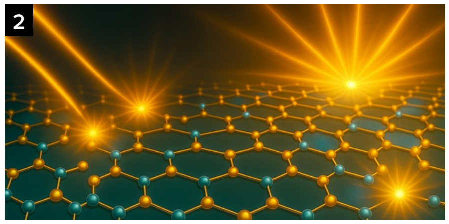
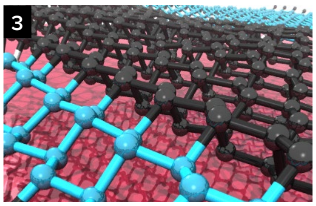
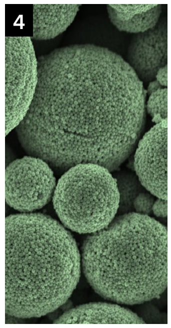
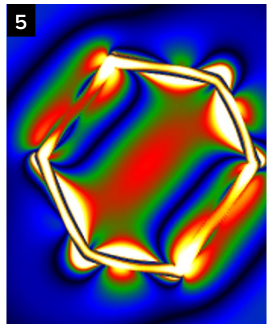
ON THE COVER











1. An atomically thin, two-dimensional layer of molybdenum disulfide (MoS_2), which can be integrated with bulk diamond for applications in diamond-based electronics, is illustrated. The image was generated by ChatGPT-5. (Nano Lett. **25**, 15353 [2025]) https://doi.org/10.1021/acs.nanolett.5c04059
2. The deterministic creation of quantum emitters in hexagonal boron nitride is illustrated. (Nanoscale **17**, 20081 [2025]) https://doi.org/10.1039/D5NR01564B
3. The strain-induced structural phase transformation of black to blue phosphorene using machine learning models is illustrated. (J. Phys. Chem. Lett. **13**, 1886 [2022]) https://doi.org/10.1021/acs.jpclett.1c03551
4. Artificial “protocells” created at Argonne’s Center for Nanoscale Materials have the ability to convert light to chemical energy through the use of a light-harvesting membrane. The image was captured with a scanning electron microscope. (Angew. Chemie **131**, 4950 [2019]) https://doi.org/10.1002/ange.201813963
5. A simulated electric field amplitude map of a hexagonal metallic nanoframe. (ACS Nano **18**, 28258 [2024]) https://doi.org/10.1021/acsnano.4c08875

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Acronyms and Abbreviations

2D	two-dimensional
3D	three-dimensional
ADR	adiabatic demagnetization refrigerator
AFM	atomic force microscopy
AI	artificial intelligence
ALCF	Argonne Leadership Computing Facility
APS	Advanced Photon Source
APS-U	Advanced Photon Source-Upgrade
AQuISS	Atomic Quantum Information Surface Science
Argonne	Argonne National Laboratory
BLAST	Bridging Length/Time Scale via Atomistic Simulation Toolkit
CL	cathodoluminescence
CNM	Center for Nanoscale Materials
CSPP	Cyber Security Program Plan
DAC	double-aberration corrected
DFT	density functional theory
DOE	U.S. Department of Energy
ESHQ	environment, safety, health, and quality assurance
FANTASTX	Fully Automated Nanoscale to Atomistic Structures from Theory and eXperiment toolkit
HEA	high-entropy alloy
HPC	high-performance computing
HXN	hard X-ray nanoprobe
IR	infrared
MIE	Major Items of Equipment
ML	machine learning
NERSC	National Energy Research Scientific Computing Center
NSRC	Nanoscale Science Research Center
PFIB	plasma-focused ion beam
PL	photoluminescence
PM	purple membrane

QET	quantum entanglement and transduction
QIS	quantum information science
QuEEN-M	Quantum Emitter Electron Nanomaterial Microscope
SEI	solid–electrolyte interface
SPE	solid-phase epitaxy
STEM	scanning transmission electron microscope
STM	scanning tunneling microscopy
TEM	transmission electron microscopy
TPCS	Transient Photoelectron and Cathodoluminescence Spectroscopy
UEM	ultrafast electron microscopy
WBG	wide-bandgap

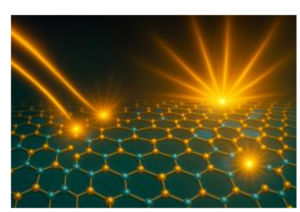
1. Introduction and Overview

Our vision for the Center for Nanoscale Materials (CNM) at Argonne National Laboratory (Argonne) is to continue its role as a world-leading research center that serves and leverages a large user science community. The basic science discoveries from the CNM impact the most pressing science and technology priorities of the United States. Our research efforts target, for example, impactful advances in microelectronics, artificial intelligence (AI)/machine learning (ML), quantum information science (QIS), and energy security. Achieving this vision requires the discovery, characterization, and integration of materials across different scales at the cutting-edge technological extremes of temporal, spatial, and energy resolutions. The complexity of this work is made possible by exceptionally capable research staff and users, combined with world-class research facilities and supporting operations staff. Staff and users work together to help determine the capabilities that are available (Figure 1-1), which span synthesis, nanofabrication, characterization, computation and theory. We work with our users to determine future capability acquisitions and anticipate emerging scientific directions in the nanosciences to support U.S. science and technology priorities.

Figure 1-1: *Integrated approach to research at CNM reflecting close links between the CNM user program, staff expertise, and state-of-the-art facilities for nanoscience and nanotechnology research to provide basic science advances that support key national scientific priorities.*

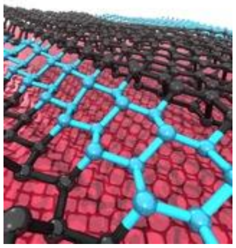
One example of our effort to support U.S. science and technology priorities is our current and planned research in microelectronics. We present throughout this document our strategy for discovering novel materials and scientific phenomena important to microelectronics. Our plans for microelectronics materials discovery are enabled by AI/ML and are coupled with advanced fabrication, characterization and computing capabilities. Our strategic focus areas in microelectronics include defect physics; novel interfaces, including two-dimensional (2D) and three-dimensional (3D) structures; transport phenomena revealed by advanced electron and synchrotron X-ray microscopy; autonomous synthesis of electronic materials; ultrafast spectroscopy to probe carrier dynamics; and novel routes for electronic switching via the control of nanomechanical structures or ferroelectricity. This work leverages unique facilities, including the Argonne Leadership Computing Facility (ALCF), the Advanced Photon Source (APS), and advanced multimodal characterization capabilities within the CNM.

Our research is organized into five cross-cutting scientific themes. These themes, described below, provide a framework for our scientific strategies that align with national science priorities:

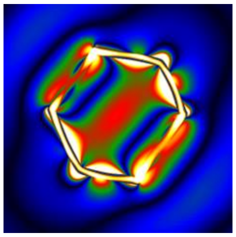


I. **Quantum Coherence by Design.** We harness CNM's expertise and capabilities in nanoscale synthesis, fabrication, characterization, and theory to discover fundamental mechanisms, novel materials, and innovative system designs for transformative insight and impact in QIS. This theme includes discovery of quantum bit (qubit) and quantum optical materials, precise placement and characterization of quantum emitters or qubits, photonic cavity control of quantum excitations, spin-photon couplings for transduction, and optically and electrically accessible defects in low-dimensional and bulk materials for the study of quantum coherence and entanglement.

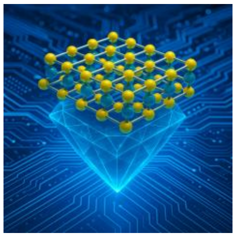
II. **AI/ML–Accelerated Analytics and Automation.** We develop AI and ML and use them to conduct multiscale simulations and real-time imaging, as well as extract information from multimodal X-ray and microscopy experiments. We further use AI/ML to perform autonomous synthesis and processing of materials. These AI/ML studies are applied to key strategic directions such as microelectronics and beyond-equilibrium systems. This theme also includes research on "digital twins"; these allow users to explore characterization experiments and conditions before they arrive at CNM so they can efficiently target the experiments most likely to succeed.



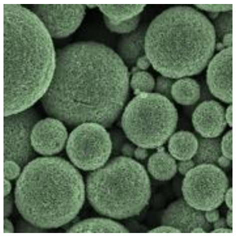
III. **Ultrafast Dynamics and Nonequilibrium Processes.** We study and control energy flow and structural changes in nanoscale materials on femtosecond-to-second timescales, spanning angstrom-to-macroscopic length scales. This work ranges from boosting microelectronic switching efficiencies using nanostructured systems to understanding fundamental steps of energy conversion. This theme leverages rapid instrumentation improvements that enable multidimensional parameter measurements, including high-resolution spatiotemporal imaging using excitations with electrons or photons.



IV. **Interfaces, Assembly, and Fabrication for Emergent Properties.** We focus on new properties that emerge from interfaces, assembly, and fabrication and are relevant to key topics such as microelectronics and QIS. The creation of emergent properties refers to behaviors that arise from materials interacting in interfaces, or through assembly and fabrication, that are not predictable based on the properties of those materials alone. New functionalities are linked to mechanical, thermal, electrical, and optical properties influenced by interfaces, assembly, and fabrication.



V. **Nanoscale Discovery for Energy.** We use CNM's expertise in computational modeling, synthesis, and advanced characterization to accelerate the discovery, research, and development of nanoscale platforms for a secure energy future. Research topics include, for example, critical materials reduction and recovery, batteries, photocatalysis, electrocatalysis, rare-earth magnets, and next-generation nano- and microelectronics.



CNM employs unique expertise and invests in unique capabilities to maximize the impact of our research efforts. This enables cross-cutting and collaborative efforts, in support of thematic research. Two examples include:

- We have invested significantly in characterization tools for materials for quantum information. Major user capabilities now include ultralow temperature cryostats equipped with microwave spectroscopies, two electron paramagnetic resonance spectroscopy tools, and extensive quantum optical microscopy tools. In Fiscal Year (FY) 2025, we brought two additional major QIS tools to users: (1) the Atomic Quantum Information Surface Science (AQuISS) lab, where we are combining quantum control (both microwave and optical) and scanning probe microscopy to enable nanometer-scale control over optically active spin quantum systems; and (2) the Quantum Emitter Electron Nanomaterial Microscope (QuEEN-M), a platform that integrates cathodoluminescence (CL) and photoluminescence (PL) spectroscopies with a probe-corrected scanning transmission electron microscope (STEM). This capability will provide new routes to deterministic placement and characterization of qubits and enable in-situ spectroscopy to characterize defect emission as a function of local structure.

- We developed a suite of cross-cutting, time-resolved electron and optical microscopies that uniquely position CNM to investigate material photophysics with a remarkable span of time and spatial scales. Beginning with the QuEEN-M mentioned above, this tool also enables time-resolved CL spectroscopy with scanning transmission electron microscopy (TEM) following highly localized, pulsed electron excitation. Faster temporal scales and larger spatial scales are accessible with the complementary Ultrafast Electron Microscope (UEM). Tabletop ultrafast optical microscopy has now been further added that can access visible through near-infrared (near-IR) probe wavelengths. These systems unlock research questions spanning localization of defect emission and photon correlations to the photoresponse of van der Waals solids. Soon, the Transient Photoelectron and Cathodoluminescence Spectroscopy (TPCS) tool will permit evaluation of electronic band structures based on angle-resolved photoelectron spectroscopy with spatial resolution of tens of nanometers. We can now examine and gain appreciable new insights into material systems spanning from single-photon emitters for quantum information to novel semiconductor devices for microelectronic switching.

We emphasize that research at CNM is frequently tied to significant capabilities at the APS and ALCF. Research collaborations among APS, ALCF, and CNM are important differentiators of CNM and are key factors in the development and implementation of our Strategic Plan. We also extend our collaborations in many cases to facilities beyond Argonne. These include DOE Leadership Computing facilities such as the National Energy Research Scientific Computing Center (NERSC), the Advanced Light Source (ALS), and the National Synchrotron Light Source (NSLS-II). Furthermore, researchers at CNM work closely with staff in many Argonne divisions across Argonne directorates.

In Section 2 of this Strategic Plan, we provide an outline of our science and technology research plans. Section 3 summarizes CNM's capabilities. This is followed by Section 4, which describes our current operations and strategic directions for enhancement, including safety, cybersecurity, data management, and staffing.

2. Science and Technology

CNM is equipped with unique and comprehensive capabilities in cleanroom-based nanofabrication; electron, X-ray, and scanning tunneling microscopies; optical and transport physics; and computational materials science. CNM staff and users conduct research consistent with our five major themes:

I. Quantum Coherence by Design,

II. AI/ML-Accelerated Analytics and Automation,

III. Ultrafast Dynamics and Nonequilibrium Processes,

IV. Interfaces, Assembly and Fabrication for Emergent Properties, and

V. Nanoscale Discovery for Energy.

Here we describe our strategic plans for each of these five themes. It is not our intent to comprehensively list all projects that could be carried out at CNM; rather we focus on our plans for strategically important research directions within the five themes. Each theme has three thrusts that provide a framework for advancing research and key basic science areas that can ultimately impact important technologies for the United States.

Theme I—Quantum Coherence by Design

Over the next five years, we will leverage the unprecedented characterization and control achieved through modern nanoscience to deepen our understanding and develop new experimental platforms for QIS. In concert with Theme II, AI/ML-Accelerated Analytics and Automation, we will create and curate large multimodal datasets to achieve unique insight into structure-function relationships of QIS systems through data-driven algorithmic approaches. Our approach to QIS research and the development of capabilities involves three thrusts: Next-Generation Quantum Systems, Control of Coherence, and Quantum Transduction.

Next-Generation Quantum Systems

The first thrust focuses on the discovery of solid-state systems that enable the creation of coherent quanta of information for sensing, computing, or communication. These systems can take many forms, such as defects or charge in a host matrix. Many of these systems are intrinsically nanoscale, and their development will benefit immensely from strategic deployment of nanoscience experimental and theoretical methodologies, expertise, and instrumentation. This thrust further addresses the need to place qubits precisely (at the nanometer level) for many QIS applications. Precise placement of qubits is one means to enable the initiation of entanglement between qubits.

In one example, we are developing a fundamentally new kind of qubit based on isolated single electrons trapped on an ultraclean solid-neon surface in vacuum (Figure 2-1) (*Nature* **605**, 46 [2022]). Using on-chip integration of an electrostatic trap and a superconducting quantum circuit, we achieved, for the first time, strong coupling between a single electron and a single microwave photon. Our single-

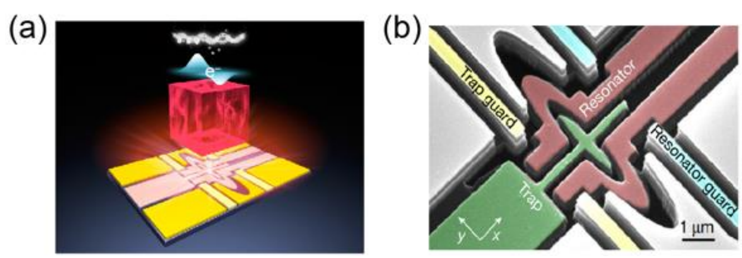


Figure 2-1: *(a) Single-electron qubit trapped on solid neon surface, interacting with a superconducting coplanar stripline resonator. (b) Scanning electron microscopy image of device around the electron trap and photon coupling region. Future work will continue to improve quantum coherence properties and entanglement to enable QIS applications (Nature* ***605****, 46 [2022]; Nature Phys.* ***20****, 116 [2024]).*

electron qubit platform takes advantage of state-of-the-art circuit quantum electrodynamics architectures to realize qubit gate control. Relaxation times and readout fidelities are already near state-of-the-art as a charge qubit. More recently, we further improved the qubit performance, reaching a record coherence time of electron qubits: T_1 and T_2 reached the 100-µs scale (*Nature Phys.* **20**, 116 [2024]). This is longer than any existing semiconducting or superconducting charge qubit. High-fidelity single-qubit gates and high-fidelity single-shot readout were also demonstrated. We further demonstrated simultaneous strong coupling of two qubits with a common resonator, an important step toward qubit entanglement and two-qubit gates.

Also within this thrust, we are developing tools newly commissioned by the U.S. Department of Energy (DOE) for QIS research, which will enable deterministic placement and detailed characterization of defect qubits of interest for quantum optics. Because all quantum emitters share the property of scale—from single atoms to several nanometers—understanding the impact of the local structural or electronic environment on the properties of quantum emitters offers technological pathways for engineered properties (e.g., deterministic emission and controlled coherence). Our QuEEN-M platform, as introduced in Section 1, integrates CL/PL spectroscopies with a probe-corrected STEM, enables real-space atomic-resolution imaging and electron energy loss spectroscopy, along with multimodal CL/PL spectroscopy with high spatiotemporal resolution through the use of ultrafast pulsers. This enables photodynamic studies of optically active defects and dopants at spatial resolution beyond the optical diffraction limit. Our goal is to ultimately reveal the complete picture of the electronic structures of quantum emitters, simultaneously with lifetime and coherence measurements. Because imaging buried quantum emitters embedded in 3D materials is so difficult, atomically thin or few-layer 2D materials will enable nanoscale CL correlative microscopy with atomic-resolution STEM; we recently demonstrated this in twisted hexagonal boron nitride (*Adv. Mater.* ***37**, e01611 [2025]*).

Progressing beyond characterization and building on our work using the Intermediate Voltage Electron Microscope–Tandem capability for carbon-ion emitter creation, QuEEN-M will be used to study in-situ formation, processing, and measurement of quantum emitters (*Nanoscale* **17**, 20081 [2025]). High-energy electron beams will be exploited to rearrange atoms in a sample (e.g., reversing the Si-carbon bond and placing of single atoms), giving atomic-scale control to what would otherwise be a recoil-driven stochastic process. Other samples (e.g., freestanding diamond membranes) will be studied for deterministic placement of nitrogen vacancy centers in diamond.

Control of Coherence

This leads to the second thrust, Control of Coherence. Coherence and entanglement rely on many details, such as relative energy levels, relative orientations of neighboring qubits, and the timescale of quantum coherence (such as spin coherence) for each qubit. Another challenge is that solid-state spin qubit research traditionally centered on defects or dopants located either in highly environmentally controlled environments or deep inside near-perfect crystals, which significantly curtails their potential utility and limits the ability to precisely control and place these systems. We are addressing this challenge via the development of the AQuISS lab, awarded by DOE for QIS research. This lab will open a new frontier in nanometer-scale control over optically active spin quantum systems by combining both microwave and optical quantum control with advanced surface science techniques such as characterization and manipulation with scanning probe microscopy, on controllable ultrahigh vacuum surfaces. In addition to near-surface bulk defects, many promising new systems can also be developed *at* surfaces (for example, surface defects, dopants, molecules, and engineered van der Waals materials).

Both the QuEEN-M and AQuISS laboratories will bring highly advanced and unique QIS capabilities to CNM users. In addition to these tools, we are leveraging our strong collaboration with the APS to develop complementary nano-focused hard X-ray microscopy capabilities that provide a unique opportunity to understand the quantum response of defects. Using CNM's unique hard X-ray nanoprobe (HXN) at the

APS, we recently developed a technique of 3D Bragg projection ptychography. Promising results already show how sound (using surface acoustic waves) can modulate defect qubits; we will use this technique extensively to build upon these results and visualize near-defect strain directly in quantum materials.

The recently completed Advanced Photon Source Upgrade (APS-U) project delivered the brightest synchrotron in the world and provided new capabilities to CNM/APS. Enabled by the 100× coherent flux increase of the APS, we will develop nano-focused X-ray excited optical luminescence detection and spectroscopy at the HXN. Data will now be collected simultaneously with diffraction-based Bragg ptychography and used to both locate optically active atomic defects (within ~10-nm precision) in 3D strain images of crystalline volumes and provide in-situ spectroscopic views of defect-level response to the local structure. Datasets from these capabilities will be organized and maintained following FAIR (findable, accessible, interoperable, repeatable) data principles to provide atomic-scale microscopy, spectroscopy, time-resolved response, and quantum state transport spectroscopy as a united data stream for AI/ML discovery of QIS materials response and engineering.

Quantum Transduction

In the final thrust, we study how quantum information can be coherently transferred from one format to another without converting to classical information. Quantum information in different excitations or formats may operate in different frequency regimes (microwave photon, optical photon, electron spin, nuclear spin, phonon, etc.); the ability to achieve quantum transduction between these formats and frequency ranges is thus an important topic in QIS. We will leverage our recent research on piezo-optomechanical transducers (*Nat. Commun.* **11**, 3237 [2020]; *Optica* **8**, 1050 [2021]), as well as various qubit systems developed at CNM, to demonstrate and study quantum transduction. Specifically, we will connect multiple CNM laboratories with QIS research via fiber-optic quantum channels to demonstrate novel remote quantum state and information transfer. The qubits will be of different varieties (e.g., quantum optical and charge-based). This work will be supported by strong theory efforts in evolving multiqubit systems in the presence of noise. We will also explore quantities such as quantum Fisher information and how to maximize it in relation to high-precision measurements and sensing. These tools will allow users to, for example, manipulate and interconnect microwave and optical qubits, enabling experimental research on new devices. Theory and simulation are essential to both enable the experimental QIS outlined in this plan and drive new experiments and directions. We will also take advantage of AI/ML based Bayesian recognition methods to accelerate challenging quantum science measurements by going beyond the statistical limits of sparse photon count-rate signals.

Theme II—AI/ML-Accelerated Analytics and Automation

Our plans in this theme center on using recent AI/ML and HPC advances for data analytics to rapidly advance materials discovery and greatly enhance information extraction from a wide range of characterization experiments. We will develop transformative theory and theory-experiment capabilities and bring them to the research community in user-friendly platforms. This leverages major computing capabilities in CNM and at Argonne, as well as user facilities across the DOE complex. The theme has three research thrusts: Multi-fidelity Scale Bridging and Materials Design, Theory Guided Information Extraction from Experimental Characterization, and Autonomous Synthesis of Nanoscale and Metastable Materials.

Multi-fidelity Scale Bridging and Materials Design

In this thrust, our diverse modeling and simulation expertise bridge the gap between the accuracy and efficiency of simulation models, while AI/ML algorithms address spatiotemporal challenges in molecular and mesoscopic simulations. Our research plans involve developing data-driven approaches to efficiently navigate high-dimensional search landscapes and significantly improving search quality, convergence speed, and scalability in material discovery and design. We will also continue to develop in-house AI/ML tools for efficient and user friendly materials design, including the Bridging Length/Time Scale via Atomistic Simulation Toolkit (BLAST; *MRS Advances* **6**, 21 [2021]), Continuous Action Space Tree search for INverse design (*npj Computational Materials* **9**, 177 [2023]), and the Fully Automated Nanoscale to Atomistic Structures from Theory and eXperiment toolkit (FANTASTX; *MRS Bulletin* **47**, 1024 [2022]). New features based on foundational models will be developed to broaden computational capabilities and functionalities. By integrating density functional theory (DFT) and ML, modeling of electrochemical surfaces and interfaces can extend beyond first-principles limitations, enable date-driven strategies for surface and interface engineering across electrodes, electrolytes, and their interfacial interactions. We will also refine user interfaces and incorporate agentic capabilities to improve accessibility for nonexperts while simplifying the integration of heterogeneous datasets to accelerate design and discovery.

We are applying ML approaches to materials discovery in technologically important materials. For example, we combine ML with first-principles computational modeling, such as with DFT, to accelerate accurate prediction of the thermodynamic and electronic properties of point and extended defects. Defects play an important role in key materials and technologies, such as semiconductors for photovoltaic, optoelectronic, microelectronic, and quantum applications. Thus, ML combined with DFT can impact these important fields. Here, native and non-native point defects control carrier concentrations and lifetimes, while extended defects (e.g., grain boundaries and dislocation cores) affect impurity segregation and carrier recombination. These effects are critical for determining power conversion efficiency. Another example is in materials for QIS applications, where the thermodynamics and charge and spin properties of defect complexes are crucial for next-generation defect qubits. DFT and ML can accurately and efficiently examine the interfacial properties (e.g., charge and spin redistribution) and inform interfacial engineering strategies for quantum coherence enhancement in solid-state qubits. This strong connection to Theme I, Quantum Coherence by Design, is an example of how our themes complement and enhance each other.

To further extend the impact of this thrust, we will leverage exascale computing (ALCF/Aurora) to resolve microelectronics-relevant defect physics across disparate length and time scales. Exascale scale-bridged simulations will enable us to connect ab-initio defect energetics, grain-boundary-mediated transport, and field-driven migration to device-level failure modes such as leakage, hot-spot localization, and electromigration. We will integrate large-scale ensembles of atomistic and mesoscopic simulations via physics-constrained surrogate models to rapidly explore design space for interconnect metals, hafnium-zirconium oxide (HZO) ferroelectric stacks, nitrides, and 3D heterointerfaces relevant to heterogeneous integration and compute-in-memory architectures. This will establish a predictive materials-to-device pipeline that informs DOE microelectronics mission needs while demonstrating exascale readiness.

Theory Guided Information Extraction from Experimental Characterization

In the second thrust for this theme, we accelerate information extraction from multimodal experimental datasets, expediting scientific discovery and using them for dynamic simulations or as training data to enhance models. This is increasingly important as experimental tools become more complex and produce more information.

An example is our recent development of a tool to automate the fusing of atomic-scale image simulations into experiments, which involve STEM and scanning tunneling microscopy (STM). “Simulation-to-experiment” comparisons can link information about mechanisms generating an experimental observation to parameters and/or specific structures used in a simulation; however, this requires mapping between the simulation and the visual or measurable expectation from experiment. To address this need, we developed Ingrained, an automated framework for image registration that allows us to fuse atomic-resolution materials imaging simulations into corresponding experimental images (*Small* **18**, 2102960 [2022]). Ingrained has been demonstrated in cases such as the grain boundaries of CdTe, the surface of pristine Cu_2O, and the surface of a 2D borophane (hydrogenated borophene). Both computational researchers and microscopists will find additional practical use cases.

This thrust is driven by innovation in advanced characterization tools that produce large datasets. Scientific user facilities are developing unique and complex tools with high data production. Locally, the CNM UEM and the CNM/APS HXN, which is capable of coherent diffraction imaging, underscore the need for more efficient information extraction. Our approach involves developing AI/ML algorithms and workflows to swiftly analyze extensive or high-dimensional multimodal data. This incorporates input from simulation models with embedded physics/chemistry models (physics-informed ML) to enable on-the-fly information extraction, facilitating real-time responses and accelerating scientific discovery. Making these capabilities available in a user-friendly framework or application is always a focus of our work in this area.

Exascale resources at ALCF will enable us to train and serve multimodal, physics-informed foundation models on large microscopy, X-ray, and transport datasets acquired from microelectronics-relevant thin films and heterostructures (more experimental microscopy efforts on this topic are described in the Interfaces for Emergent Properties section). These workflows will move beyond post-processing, enabling near-real-time inference during beamtime and microscopy sessions to steer experiments toward defect-rich or kinetically active regions. In microelectronics, this will allow extraction of causal links between voids, dislocations, trap states, and field-dependent device degradation, accelerating qualification pathways for emerging ferroelectric, 2D, and wide-bandgap (WBG) platforms. By coupling exascale inference with in-situ acquisition, we create a closed-loop characterization and simulation environment within which to reliably screen and predict lifetime modeling in manufacturing-relevant conditions.

Autonomous Synthesis of Nanoscale and Metastable Materials

For the third thrust, we will establish AI-guided infrastructure that empowers users to autonomously control metastability across diverse length scales—from single atoms to nanoscopic domains and mesoscale morphology (*Chem. Mater.* **35**, 3046 [2022]). We will establish a state-of-the-art experimental paradigm that leverages connected modular robotics, human-machine interfaces, and AI/ML-driven decision intelligence. The goal is to efficiently search large, complex parameter spaces for emerging classes of nanomaterials discovery, often under the constraints of limited experimental data.

One example in this thrust is PolyBot (*Chem. Mater.* **35**, 3046 [2023]), an AI/ML-integrated modular robotic material discovery platform we developed to perform closed-loop synthesis, processing, characterization, and optimization of novel materials, including electronic polymers (*Nat. Commun*. **16**, 1498 [2025]) and neuromorphic materials (Figure 2-2). Over the next five years, we will continue upgrading this autonomous materials platform with additional adaptive AI decision-making and experimental capabilities for staff and user projects. More importantly, we will use this newly developed platform to accelerate the discovery of electronic functional polymers for electronics, peptides with desired sequences, and inorganic nanoparticles with desired properties. In the coming years we expect fruitful development of robust and stretchable polymeric materials to be used as sensors for medical diagnostics and other applications.

Figure 2-2: *Electronic polymer synthesis platform of Polybot, an AI-integrated robotic synthesis laboratory (Chem. Mater.* ***35****, 3046 [2023]).*

We will also leverage exascale computing and reinforcement learning to guide autonomous synthesis toward discovery and control of microelectronics-relevant metastable states that are otherwise experimentally inaccessible. Large-scale digital twins of synthesis (polymer casting, ALD, solution growth, pulsed lithiation, etc.) will be executed to prescreen conditions and feed into robotic decision-making on

PolyBot and related autonomous platforms. In microelectronics, we will target discovery of robust interfacial adhesion layers, low-κ dielectrics, neuromorphic oxide states, and stretchable polymer conductors for heterogeneous integration. Exascale policy learning, coupled with robotic execution, enables AI-driven materials manufacturing that closes the design-to-device loop.

Theme III—Ultrafast Dynamics and Nonequilibrium Processes

All operational devices experience nonequilibrium phenomena and may undergo processes such as electron-electron scattering, photon or phonon emission, local structural or crystal phase changes, and macroscopic mechanical motion and ordering/disordering. To increase the performance and efficiency of devices and uncover entirely novel phenomena that might be exploited, it is vital to understand steps ranging from the introduction of energy to how energy evolves and is redistributed. CNM staff and users work to understand the temporal evolution of metastable materials and lattice phase changes, nonequilibrium mechanical responses, plasmonic processes, and the dynamics of the interaction of materials with various excitation quanta (optical, magnetic, or electronic).

At CNM we both maintain and develop capabilities that allow us to investigate carrier mobility and loss mechanisms in microelectronics, photon correlations in quantum information materials such as novel defects, photon capture in plasmonic materials for hot electron photocatalysis, and discovery of nonequilibrium phases of matter. We use spatiotemporal tools that can span 15 orders of magnitude in time and 6 orders of magnitude in space at high sensitivity. Over the next five years, we will offer new tools, methods, and approaches to target central problems in condensed matter physics, novel optical phenomena, and chemical processes, with impacts on novel functionality, including on catalysis, energy conversion, and the circular economy. We will focus on three thrust areas: Optical and Carrier Dynamics in Nanomaterials, Engineered and Responsive Dynamics of Strain and Mechanical Motion, and Dynamics of Ordering and Response of Hierarchical Assemblies.

Optical and Carrier Dynamics in Nanomaterials

Our plans in the first thrust center on the fact that many prospective technologies rely on controlling a material's optical properties and electrical charges to achieve a particular functionality (e.g., photon detection, optical switching, or laser emission). Nanoscience has a key role to play here, because nanostructuring offers additional tools to control optoelectronic properties that are affected by the size, shape, and composition of nanomaterials.

As an example, we continue to study the rich chemistry and physics of colloidal semiconductor quantum wells. Colloidal nanoplatelets have narrow, thickness- and composition-dependent intraband transitions (*Nano Letters* ***25***, 2366 [2025]). In addition to ultrafast switching (U.S. Patent 11,333,908), the tunable intraband transitions are engineered to produce single-carrier, thresholdless, near-IR optical gain (Figure 2-3; *ACS Photonics* ***11***, 3991 [2024]; Patent Assignment 17/676,307). This will be a very active area of research for the next several years in CNM.

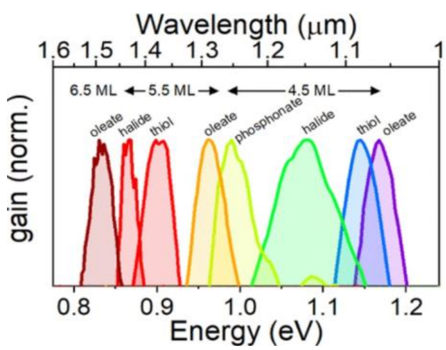


Figure 2-3: *Near-IR optical gain from intersubband transitions in CdSe nanoplatelets. Gain position is tunable via nanostructure monolayer thickness and surface passivation (*ACS Photonics ***11****, 3991 [2024]).*

In this thrust, we further explore the dependence of the nanomaterial dynamics on dielectric and deposition conditions, including the self-assembly of nanoparticles into larger structures and the dependence of optical properties on collective processes such as phonons. We continue to probe the influence of exciton dynamics in these materials on their single-photon emission properties, which are highly relevant to quantum optics (*Phys. Rev. Mater.* **5**, L051601 [2021]). This is in collaboration with research efforts in Theme I, Quantum Coherence by Design.

Engineered and Responsive Dynamics of Strain and Mechanical Motion

Within this thrust, we understand, predict, and control the behavior of nanoscale mechanical structures for applications ranging from microelectronics to novel architectures enabled by kirigami (*PNAS* **122**, e2425200122, [2025]). Structural deformation—governed by thickness, surface termination, and defects such as dislocations—can fundamentally alter mechanical response at the nanoscale relative to bulk, opening opportunities for new functional properties. Realizing these opportunities requires a predictive understanding of dynamically driven nanostructures.

We will pursue coordinated theoretical and experimental efforts that integrate multiscale materials modeling and inverse design with ultrasensitive dynamical characterization to probe mechanical behavior at the nanoscale. These studies elucidate and control couplings among light, matter, and phonons, including how interacting and mode-coupled nanomechanical oscillators shape optical responses.

Dynamics of Ordering and Response of Hierarchical Assemblies

In the third thrust, we probe structural evolution and internal particle dynamics in nonequilibrium nanoscale systems and their macroscopic impacts. Systems include those driven by external fields, chemical potential, or near-phase transitions. We will integrate real- and reciprocal-space imaging with molecular dynamics and AI to study biomimetic peptides, self-assembled colloids, and complex fluids. Probing nonequilibrium processes requires in-situ probes that can measure structure and dynamics simultaneously. Thus, we are further expanding our collaboration with APS-U Sectors 8 and 9 to use coherent X-ray scattering techniques to understand the particle dynamics. With coherent flux in the range of 5×10^{13} photons/second, we will reach unprecedented length scales of 5 microseconds to 1 nm and time scales of 10 nanoseconds to 1,000 seconds. Many sample environments cand be studied utilizing available shear cells, microfluidic flow cells and high-pressure cells (*J. Phys. Chem. B* **127**, 7408 [2023]; *Phys. Rev. Lett.* **134**, 178202 [2025]).

Our goal is to continuously update our experimental research capabilities to build upon our strong, productive, and traditional efforts in ultrafast optical physics, which benefit from our current range of time-resolved contrast mechanisms, such as optical photons for electronic transitions, IR photons for vibrational modes, terahertz photons for transient conductivity, or X-ray photons for structural dynamics. We also seek to continue to develop our optical microscopy capabilities that provide spatial resolution with dynamic capabilities. This will complement the dynamic spectroscopy capabilities currently present, which we will develop further for electrons and X-rays via, respectively, the UEM and HXN. The plans for optical, electron, and X-ray dynamics are described below.

Samples with small lateral extent or spatially varying samples with inhomogeneities or variations in electronic properties make capabilities such as ultrafast optical microscopy useful. Inhomogeneities can play key roles in the local nucleation and triggering of events (e.g., phase changes) and may present atypical charge separation or energy funneling. Characterizing the time scale and channels into which energy flows upon impulsive excitation is fundamental to a wide range of nonequilibrium phenomena. Fourier plane imaging approaches permit examination of mechanical motion, such as phonon generation and thermal dissipation, which can otherwise be challenging to evaluate because electron–phonon scattering can occur on femtosecond to picosecond time scales. Our interest here lies in gaining a fundamental understanding and control of dynamic electron–phonon processes, with broader goals of tailoring energy flow within nanostructured materials and controlling spectral evolution of carriers and phonons. Concomitantly, we will perform theoretical modeling of nonequilibrium electron–phonon dynamics, using a combination of many-body perturbation theory, Boltzmann transport equation, time-dependent DFT, and first-principles molecular dynamics. We aim to understand how electron–phonon dynamics are impacted by nanoscale heterogeneity, anisotropy, interfaces, and proximal phase transitions.

Transient electron microscopy tools (e.g., UEM, QuEEN-M, and DAC STEM) will evaluate sample changes spatially (with sub-nanometer resolution) and temporally to assess real-space local structure, reciprocal space (via electron diffraction), charge distribution, and local electric field on ultrafast time scales (see, for example, Figure 2-4). By flexibly tuning these microscopic contrast mechanisms at a fixed time slice relative to a dynamic process, the UEM can deliver insights on ultrafast structural and chemical changes to a wide range of systems.

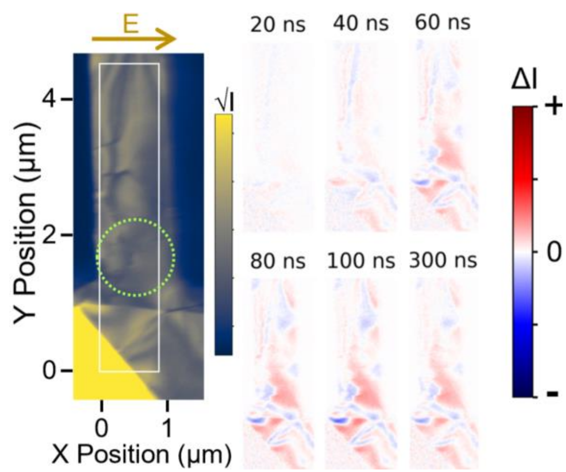


Figure 2-4: *Voltage-pulse-induced defection of a suspended TaS_2 flake monitored with UEM (arXiv:2306.01171v1).*

Because it is so complex, this type of system was previously available to only a few research groups that specialized in technique development. Now, however, we can harness this investment's potential on behalf of a broad user community and staff, advancing many areas of nanoscience in parallel through the improved understanding of transient processes. These transient processes include exciton localization, short-lived metastable phases, photo-induced segregation, dynamics in topological materials, carrier dynamics, plasmonic systems, molecular motors, and magnetic fluctuations.

We are developing novel sample environments and routes of sample excitation that are relevant for both fundamental science and devices. For example, we are working to make ultrafast mechanical and electrical triggering accessible in the UEM, as well as a variable-delay pump-pump-probe mode. Combined with ultrafast probing, this will permit insights into nonequilibrium phenomena in an electric field and under strain. Structural distortions that exist upon formation and disturbance of quantum material systems will be targeted, as will in-operando nano-enabled transistors, memories, nanoelectromechanical system behavior, and microstructure response to high strain rates.

Theme IV—Interfaces, Assembly, and Fabrication for Emergent Properties

A central motive for this theme is that interfaces frequently play an important role in the optical, electronic, and mechanical properties of materials. Furthermore, interfaces, assemblies, and fabricated nanostructures can be the central feature for a desired functionality, such as long-lived charge separation across an interface. CNM's expertise in assembly and fabrication, combined with unique theory and characterization capabilities, provides an excellent opportunity for CNM scientists and users to create, understand, and ultimately control interfaces for a desired property or function. We approach this challenge through three thrusts: Interfaces for Emergent Properties, Assembly for Emergent Properties, and Fabrication for Emergent Properties.

Interfaces for Emergent Properties

In this thrust, we design strategies for fabricating varied (hetero) interfaces that showcase enhanced functionalities across domains. We will use advanced in-situ and ex-situ probing techniques at the atomic scale, as well as computational and theoretical approaches including an AI model to predict electronic, thermal, and mechanical properties at interfaces and with varying defect distributions. Examples of heterointerfaces include mixed dimensional (2D/3D) structures.

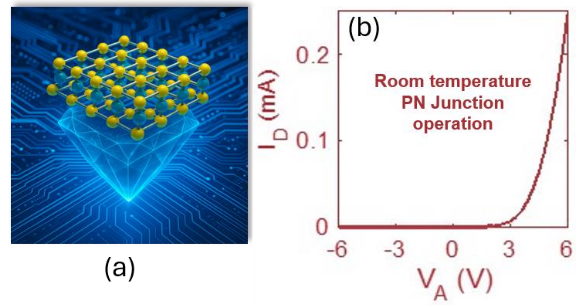


Figure 2-5: *(a) Formation of 2D/3D heterojunction via stacking of n-MoS2 on P-diamond and (b) measuring I-V characteristics of the device demonstrating excellent rectification performance at room temperature (Nano Lett.* ***25****, 15353 [2025]).*

In one recent example, we fabricated a 2D/3D heterojunction using p-doped diamond and n-doped MoS_2 (Figure 2-5). This demonstrates PN junction with excellent rectification performance and a record high-current density at room temperature, mitigating a longstanding bottleneck in achieving n-type doping in diamond (*Nano Lett.* **25**, 15353 [2025]). This opens new avenues to develop diamond-based electronics through heterointegration with 2D-transition metal dichalcogenides (TMDCs) and other semiconductor materials.

Understanding the interfacial charge transfer mechanisms, the role of defects, and strain at the interface will be crucial for controlling and manipulating TMDC systems. We will leverage our unique TEM capabilities to study how structural defects and interfaces at the atomic scale influence electronic properties and failure in electronic materials and devices. We are implementing a range of modes to enable multimodal imaging around defects and interfaces for correlating local structure and properties (e.g., scanning nanodiffraction [four-dimensional TEM] for mapping strain and crystal structure, phase imaging approaches for mapping local electric fields, and integrated optical and electron spectroscopy for imaging electronic and chemical variations). These allow us to visualize a variety of defects, such as dislocations, stacking faults, grain boundaries, and trap states as well as interface roughness and chemical segregation.

Our capabilities for in-situ TEM under heat and/or electrical bias allow us to visualize defect-mediated switching or failure processes, such as filament nucleation, vacancy migration, or interface degradation. We will continue to develop time-resolved TEM imaging and spectroscopy, using fast cameras and pulsed electron beams to observe transient defect dynamics and structural rearrangements on nanosecond to millisecond timescales (e.g., time-resolved electron-energy loss spectroscopy (EELS) to track electronic and chemical phenomena such as chemical bonding, oxidation state/vacancies, or carrier localization during breakdown).

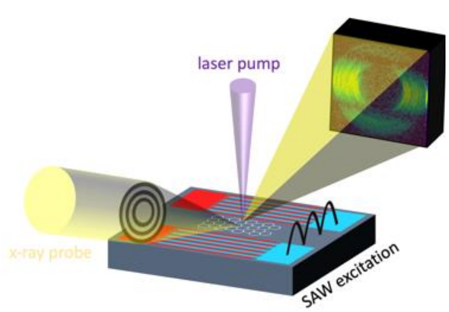


Figure 2-6: *Surface acoustic wave-laser pump X-ray probe experiment.*

Another important new direction will be leveraging AI to obtain the required large statistics for understanding defect-property relationships (e.g., autonomous/high-throughput TEM experiments and defect identification, classification, and tracking). We will apply these to a range of defect and interface-driven phenomena in microelectronics, in collaboration with the AI/ML-Accelerated Analytics and Automation theme.

Other plans include using HXN to perform time-resolved strain microscopy at interfaces by exciting surface acoustic waves to modulate strain (Figure 2-6). Of particular interest are 2D materials with tunable optoelectronic properties, particularly through piezoelectric effects. We will examine defects that lead to dielectric breakdown in WBG semiconductors such as Ga_2O_3, diamond, SiC, and their heterostructures. We will also examine the nature and evolution of metal/dielectric interfaces. For instance, we recently applied multimodal TEM approaches to elucidate the role of a nanometer-scale oxide interlayer on the function of hafnia-zirconia–based ferroelectric capacitors (*ACS Appl. Mat. Int.* **16**, 68562 [2024]). These studies will provide not only mechanistic understanding but also design guidelines for engineering more robust materials and interfaces for electronics applications.

On the mechanical interfaces, we will continue studies to understand energy dissipation at tribological interfaces that include high-entropy alloys (HEAs) and the MXene family. We recently demonstrated ultralow friction and wear at ambient conditions in HEA $(MoWNbTaV)_{0.2}S_2$ synthesized in a 2D configuration (*Small* **21**, 2500322 [2025]). Our experimental studies coupled with molecular dynamics (MD) simulations revealed that the presence of Mo triggers tribocatalytic activity under high contact pressures, resulting in extended lubricant lifespan during tribological test. We will explore this tribocatalytic effect in other HEA MXenes to answer fundamental questions on maintaining superlubricity for an extended time.

Assembly for Emergent Properties

In this thrust, we examine how functional material assemblies interact across interfaces to produce emergent physical and biological behaviors. Building on our established bioelectronic nano–bio interfaces for non-invasive neural stimulation using X-ray–activated nanoscintillators (*ACS Nano* **15**, 5201 [2021]) and on magnetically coupled nano–bio systems (*J. Am. Chem. Soc.* 2c10749 [2022]), we will develop ferromagnetic lithography–defined architectures that create dynamic interfaces with cartilage tissue. These model systems will enable controlled mechanotransduction studies, in which magnetic and electronic stimuli modulate biological signal pathways. This will inform the design of multifunctional bioelectronic materials that integrate magnetic, electronic, and biological functions to enable controllable signal transduction and adaptive biological responses.

In future work for this thrust, we will target novel approaches to the assembly of varied 2D and 3D materials that show interesting electronic properties and are of great potential relevance to microelectronics. We will leverage unique characterization facilities at CNM and APS to probe the structural and electronic properties of the 2D/3D materials interfaces to understand the fundamental mechanism of charge transport. We will also use in-situ TEM to correlate the transport properties of devices made from multilayer structures. In efforts connected with Theme II, AI/ML-Accelerated Analytics and Automation, we will pursue an optimized algorithm for data reconstruction to better understand the interface structure in 3D/2D heterostructures.

Fabrication for Emergent Properties

In this thrust, we manipulate materials or systems to exploit emergent phenomena for specific purposes (e.g., mechanical, plasmonic, or quantum applications). The focus is to advance our understanding of material interfaces to enable guided improvement of the functions of the system or realization of entirely new phenomena. We will work toward photo-electrostatic control of charge dynamics at interfaces between 2D materials and 3D WBG materials. The distinctive characteristics of 3D WBG materials (e.g., their polar surfaces, defect-driven Fermi-level pinning, and band-edge tunability) offer versatile routes for controlling interfacial charge transfer and recombination processes. This approach will both deepen our fundamental understanding of charge dynamics across atomically sharp interfaces and pave the way for photo-actuated low-power electronics, high-efficiency optoelectronics, and quantum photonic devices. A key methodological strength of this project is its glovebox-based in-situ 2D transfer setup coupled with multimodal spectroscopy, which is crucial for preserving the intrinsic properties of air-sensitive, high-mobility 2D semiconductors such as InSe and SnS_2. By combining deterministic 2D stacking with in-situ atomic force microscopy (AFM), Raman, and PL measurements, we will capture pristine interfacial states and monitor charge-transfer mechanisms in real time without ambient degradation. Through this photo-electrostatic framework, we will establish a new class of functional interfaces that enable reconfigurable charge transport and tunable optical/electronic coupling, setting the foundation for next-generation, energy-efficient, quantum-enabled device architectures.

In another example, we propose a mask-free, damage-free route to create ferroelectric memories. Selective solid-phase epitaxy (SPE) crystallizes ferroelectric and WBG oxides only inside sub-10-nm apertures in robust dielectrics (SiN/SiO_2/AlN), yielding orientation-controlled single crystals and true 3D stacks with back end of line-compatible localized anneals. Nanoscale confinement generates large strain/strain-gradients that strengthen ferroelectricity and deterministically template domain architectures. The platform targets ultra-dense ferroelectric tunnel junction and ferroelectric field-effect transistor memories (~1–10 Tb/in^2), negative-capacitance field-effect transistors for steep-slope logic, and ferroelectric-gated β-Ga_2O_3/WBG devices. We also stack nanopatterned oxides with 2D materials to program band structure, carrier density, and Moiré/strain fields at ~10 nm for reconfigurable nano-optoelectronics.

Theme V—Nanoscale Discovery for Energy

In this theme, we leverage our leadership in nanomaterial synthesis, state-of-the-art experimental characterization and computational modeling to advance basic science and technologies relevant to energy security and critical materials. This thematic research has three major thrusts: Critical Materials for Energy Security, Nanoscience for Next-Generation Energy Technologies, and Energy-Efficient Microelectronics. We outline below the ways we are addressing these thrusts through staff and collaborative user research.

Critical Materials for Energy Security

Many of the materials currently necessary to maintain control of energy destiny are rare. The demand for these materials is projected to increase significantly over the coming decade, whereas the supply of these resources will be limited by a myriad of challenges. In this thrust, we work to reduce the use of critical elements in catalysts, battery materials, and magnets, and to design new materials and in situ analytical tools to recover critical materials.

To replace or minimize the use of critical materials we will investigate earth-abundant electrocatalysts. For example, we are taking steps to replace iridium for the oxygen evolution reaction in a proton exchange membrane water electrolyzer. This involves implementing a cobalt spinel catalyst co-doped with lanthanum and manganese prepared from a zeolitic imidazolate framework. It has demonstrated great activity and stability in acidic environments (*Science* **380**, 609 [2023]). By investigating nickel aluminum layered double hydroxides (NiAl-LDHs) with different interlayer anions (CO_3^{2-}, Cl^-, and Br^-) with multiple characterization techniques and DFT, we showed that the interaction between ions in the alkaline electrolyte and electrode materials plays a critical role in optimizing water electrolysis performance (*ACS Appl. Mat. Int.* **17**, 28, 41271 [2025]). To reduce precious metals in water electrolyzers while maintaining their performance, we used common industrial processes to fabricate Ir-Co_3O_4 electrocatalysts with different structures of iridium oxide over cobalt oxide nanocrystals. In situ characterization shows that the structure containing two atomic layers of IrO_x is highly ordered, remains stable under oxygen evolution reaction conditions, and reduces the amount of iridium (*J. Am. Chem. Soc.* **147**, 7008 [2025]).

Looking forward, we are developing synthetic strategies to create HEA nanoparticles (>4 elements) as catalysts (*ACS Nanoscience Au* **5**, 407 [2025]). HEAs allow fine-tuning of catalytic activity at the atomic level to enhance performance while reducing use of precious metals. To tackle the vast compositional parameter space, we are combining CNM's robotic synthesis platforms with a fluorescence-based optical screening technique to evaluate numerous catalysts in a single experiment as shown in Figure 2-7; this approach will enable comprehensive study of HEA catalytic behavior, with AI models analyzing the generated dataset.

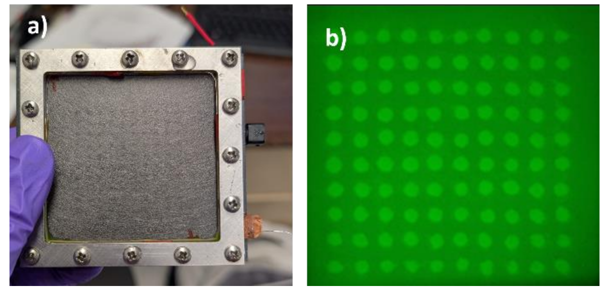


Figure 2-7: *(a) Optical screening cell for catalyst activity developed at CNM. (b) Fluorescence images captured under electrochemical testing conditions for Pt nanoparticles.*

We also will minimize critical material (e.g., Nd, Sm) use in high-performance rare-earth magnets while maintaining magnetic strength by establishing structure-property relationships in these materials. By correlating Lorentz 4D-STEM magnetic maps with atomic-scale structural and compositional data, we will uncover how chemistry, defects, and grain boundaries control magnetization, coercivity, and exchange pinning. Combined with micromagnetic modeling, these insights will identify key mechanisms and design pathways to achieve high performance with reduced rare-earth usage.

It is also crucial to develop strategies for recapturing critical materials in waste streams. A recent project used CNM's inductively coupled plasma optical emission spectroscopy system to understand interfacial ion transport during liquid-liquid extraction process (*PNAS* **121**, e2315584121 [2024]). We will design porous and layered materials that are capable of selective controlled absorption and release specific metal ions. For example, 2D materials—including graphene, metal-organic frameworks, and MXene—with tailored nanoplate structure and tunable porosity exhibit adjustable physical confinement and surface charge, which can be engineered to enhance ion transport kinetics and separation selectivity. Selective recovery can be enhanced by applying external potentials that exploit distinct redox windows (for example, Ni, Co) associated with different critical elements. Moreover, the newly installed near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) at CNM will enable in situ monitoring of surface-sensitive chemical analysis under conditions that closely mimic reaction environments.

We also recently investigated selective Pb^{2+} extraction using functionalized electrodes in capacitive deionization (*Water Research* **268**, Part B, 122665 [2025]) in collaboration with University of Chicago. Using DFT simulations, we determined the affinity and selectivity of functional groups for various ions. We are now applying this technique to extract lithium ions (Li^+) from aqueous solutions. High-throughput DFT calculations and ML are being used to design capacitive deionization electrode surface chemistry for enhanced Li^+ selectivity. This approach will create efficient surfaces for reversible Li^+ adsorption and desorption, contributing to lithium recovery for battery applications.

Based on our experience and success in developing peptide materials that were designed to bind biological cofactors like heme, new peptides will be investigated for high affinity/high specificity with rare earth elements (*Biomacromolecules* **25**, 3398 (2024]). A combination of simulation and high-throughput experimentation generating a database of sequence specific binders will enable ML-fueled prediction of novel materials for critical materials separation and recovery similar to our ML investigations that employed IR spectroscopic input to aid in sequence prediction for pentapeptide self-assembly (*Sci. Adv.* **11**, eadt9466 [2025]). These materials are complementary to current user investigations employing radiolabeled rare earth elements bound to peptides for targeted therapies like prostate cancer.

Nanoscience for Next-Generation Energy Technologies

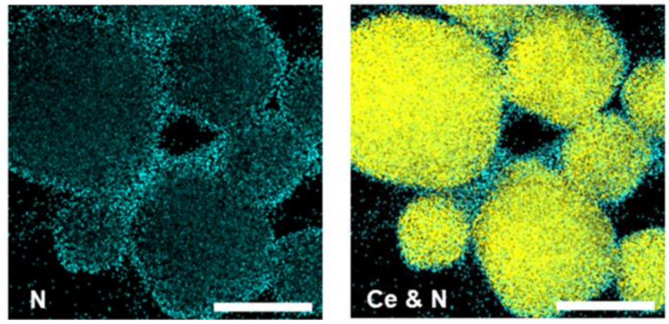


Figure 2-8: *TEM−EDS mapping of CeO_2-PM. Distinct nitrogen signals at the edges of the nano-bio hybrid indicate the presence of immobilized protein patches on the surface of ceria (scale bar = 500 nm).*

In this thrust, we focus on using synthetic and characterization capabilities to unravel the underlying science at the nanoscale to develop next-generation energy technologies. In collaboration with APS and our users, we employed advanced synchrotron techniques and 3D electron diffraction to elucidate the structural degradation mechanisms of single-crystalline, Li-rich oxide cathodes (*Science* **606**, 384–392, [2024]). By understanding the underlying mechanism, we collaborated to design novel cathodes with compositional and structural dual gradients, enabling ultra-stable battery performance (*Nature Energy* **9**, 1252 [2024]). Through multiscale diffraction and imaging, we revealed that air exposure induces surface structural distortions and a transition to a metastable O1* phase, which are primarily responsible for the electrochemical degradation (*Nat. Comm.* **16**, 6519 [2025]). By combining single-atom STEM-EELS with CL, we studied the distribution and valence state of single-atom dopants on CeO_2 (Figure 2-8)—serving as catalysts for CO_2 methanation—where CL provided chemical information inaccessible to EELS due to the dopants' trace amounts (*ACS Appl. Mat. Int.* **17**, 29695 [2025]).

We will continue integrating in-situ multiscale imaging and diffraction characterization—including atomic-resolution TEM, nanometer-scale analysis, and full-cell measurements—to obtain a comprehensive understanding of battery materials and their structural and strain evolution during operation. By combining low-temperature TEM sample preparation and air-free transfer techniques with low-dose imaging and spectroscopy, we will also directly study the solid–electrolyte interface (SEI) and interphase evolution under realistic operating conditions. This approach will allow us to capture delicate, beam-sensitive structures and chemical changes at the SEI, providing critical insights into the formation, stability, and degradation mechanisms that control next-generation battery performance and lifetime.

We will also use HXN to advance understanding of energy materials under realistic conditions. The nanofocused beam enables simultaneous mapping of structure, strain, composition and chemical state within working battery electrodes, interfaces, and catalysts at tens-of-nanometers spatial resolution. Building on our recent progress in nanodiffraction studies of Li-ion battery materials (*Nat. Comm.* **16**, 6519 [2025]; *Nat. Comm.* **16**, 434 [2025]; *Nat. Energy* **9**, 1252 [2024]), we will address sodium-ion batteries and Ni-rich cathodes, which will reduce reliance on critical materials such as lithium, cobalt, and manganese.

We will develop new environmental sample stages that integrate gas, liquid, temperature, and electrical control for operando electrochemical and catalytic experiments. These platforms will allow direct observation of charge storage processes, interphase formation, and electrochemical reactions in batteries, fuel cells, and CO_2 reduction systems. We will extend the multi-crystal rocking-curve method (*Science* **384**, 912 [2024]) to capture both statistical and individual lattice distortions over hundreds of nanoparticles in situ. By combining nanodiffraction, nanoscale X-ray fluorescence, and nano-X-ray absorption near edge structure spectroscopy, we will correlate local redox, strain, and defect evolution that govern material efficiency and lifetime.

We also advanced photon-driven redox catalysis without reliance on Pt, Pd, or other precious metals through hierarchical nano-bio architectures that integrate semiconductor structures with archaeal purple membranes (PMs). We demonstrated a CeO_2-PM hybrid catalyst capable of abiotic nitrogen-to-ammonia conversion accompanied by selective glycerol oxidation under ambient conditions (*J. Am. Chem. Soc*. **147**, 34477, [2025]), revealing that directionally aligned membrane patches can inject photoexcited charges into the inorganic semiconductor CeO_2 to extend carrier lifetime and drive multielectron reactions via proton-coupled electron transfer. Advanced electron microscopy, synchrotron scattering, transient absorption spectroscopy, and magnetic-resonance spectroscopy confirmed reproducible redox activity and long-lived charge carriers.

Moving forward, we will develop semiconductor plate-like layered architectures interfaced with archaeal PMs to mimic enzymatic redox chemistries within solid-state environments. These hybrid systems will be explored for photochemical generation of H_2O_2 and selective glycerol oxidation as model reactions to study coupled redox processes. We will employ XPS, UPS, TEM, AFM, CL, transient absorption, and complete synchrotron grazing incidence small- and wide-angle X-ray spectroscopy studies to resolve interfacial electronic structure, excited-state charge dynamics, light–matter coupling, and nanoscale morphology. Understanding how these factors direct selective two- and four-electron steps will establish the fundamental principles of photon-driven redox catalysis under ambient conditions and guide the development of next-generation catalytic materials.

Energy-Efficient Microelectronics

In this thrust, we focus on understanding materials and phenomena to help develop next-generation microelectronics. Van der Waals multiferroic materials hold transformative potential for the next generation of multifunctional micro- and nanoelectronics. For example, recent non-centrosymmetric layered tin selenide (SnSe) with AA-stacked structure has revealed room-temperature multiferroicity (*Nat. Comm.* **16**, 3648 [2025]). Unlike the typical centrosymmetric AB stacking, this configuration breaks inversion symmetry across multiple layers, enabling the coexistence and coupling of in-plane and out-of-plane ferroelectric polarizations. This makes it possible to manipulate one polarization component via the other using minimal electric fields, resulting in ultra-low-voltage switching (~0.28 V) which scales favorably with layer thickness. Complementary electron microscopy reveals coexisting armchair- and zigzag-type ferroelastic domains (Figure 2-9), experimentally confirming the theoretically predicted degenerate ground states and demonstrating the coexistence of ferroelectric and ferroelastic orders. Non-centrosymmetric SnSe represents the first 2D layered multiferroic system stable at ambient conditions. Future work will connect with AI/ML and interface research in other themes to explore modulating the domains with twisted layering and solve the atomic structure in these twisted structures through electron microscopy. Going forward, we will focus on further developing this and similar systems as versatile platforms for energy-efficient, reconfigurable, and multistate nanoelectronic and microelectronic devices.

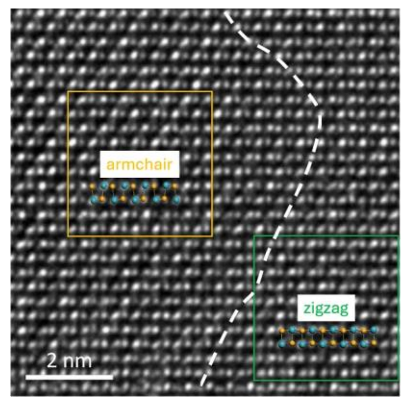


Figure 2-9: *Side-view HR-TEM image. Yellow box: typical (010) type (armchair) configuration. Green box: (100) type (zigzag) configuration. White dashed line: guide for the eye indicates domain boundary (Nat. Comm.* ***16****, 3648 [2025]).*

3. Capabilities

CNM provides an array of capabilities and expertise to its users. These include optical spectroscopy from ultraviolet to terahertz at the extremes of spatial and time resolution; a suite of electron microscopes with a wide range of capabilities that include the UEM; a full suite of variable-temperature scanning tunneling microscope capabilities; comprehensive nanofabrication capabilities in a newly expanded 18,000-ft^2 cleanroom; the Carbon supercomputing cluster, which is being upgraded specifically for data-intensive AI/ML workloads; quantum science capabilities designed to study single-photon as well as charge- and spin-based coherent systems; and HXN, jointly operated by CNM and APS. The CNM "Tools & Capabilities" page provides a complete list and description of all CNM capabilities. For additional details, please see **Appendix 1.**

Our approach to upgrading our toolset begins with continuously analyzing the suite of capabilities available to users. New instruments and enhancements are added as needed. We also remove capabilities that have become obsolete or are used infrequently or not at all. Our primary mechanism to upgrade our toolset is the recapitalization of a portion of our yearly funds. We have also acquired equipment through Nanoscale Science Research Center (NSRC) QIS grants and NSRC Major Items of Equipment (MIE) project.

Recapitalization refers to the use of up to 10% of CNM annual operating funds each year to procure new tools or to upgrade aging tools. It is the mechanism that enables the largest quantity of new tools and upgrades each year. Our process for recapitalization incorporates suggestions from users and staff.

We have also acquired new capabilities through three NSRC QIS grants. The first, "Photon qubit entanglement and transduction," provided major new capabilities in quantum optics, enabling time-correlated single-photon counting microscopes in both the visible and near-IR regimes. The near-IR microscope includes single-photon detectors of ultrahigh-efficiency superconducting nanowires. In addition, we constructed a magneto-optical microscope that is equipped with a microscope cryostat and performs spin-dependent optical emission studies of quantum materials. The equipment from the other two grants, as well as the planned scientific and user impact, were described in Theme I, Quantum Coherence by Design. Each of these tools became available to users in FY 2025.

The NSRC MIE project extends across all five NSRCs and represents a major DOE commitment to further the nation's capabilities in nanoscience research. The $80 million project enables investment in major capabilities that are too large to be accommodated through NSRC recapitalization funds. By FY 2026, CNM will have acquired four new tools via this project. The dynamic double-aberration corrected (DAC) STEM and the TPCS tool will significantly enhance our nanoscale dynamics research capabilities. The dynamic DAC-STEM's higher spatial resolution complements the UEM but will have longer time-scale dynamics capabilities (tens of microseconds and beyond). The TPCS tool will be placed in APS Sector 29, with a vacuum highway between the TPCS and other beamline tools to enable the same sample to be studied for structure and dynamic function correlations. The TPCS tool continues our effort to study dynamics with different contrast mechanisms. Because this tool can directly extract carrier energy dynamics, it will complement our time-resolved optical capabilities when the optical spectrum is too dense with many transitions, or in systems that lack significant optical extension such that time-resolved optical studies are not possible. A newly acquired plasma-focused ion beam (PFIB) will enable nanostructuring without concern for gallium-ion doping issues, which can limit electronic performance of a nanostructured device. It also enables much faster materials preparation for TEM studies. Finally, the milliKelvin scanning-tunneling microscope (mK-STM) gives our users access to millikelvin temperatures, complementing our other variable temperature STMs and enabling detailed quantum- and spin-state STM studies that were previously impossible. As of December 2025, the PFIB and mK-STM have already been installed at CNM. The DAC-STEM and TPCS tool will be installed in 2026.

4. Operations

Here, we briefly outline our plans for key operations areas, particularly staffing, safety, cybersecurity, and data management.

Staffing

CNM opened for operations and began welcoming users in the fall of 2006. Since then, CNM has grown as a facility, with approximately 44 regular staff (research and technical support) members and 1,000 users annually. We provide an up-to-date, detailed version of the CNM Organizational Chart on our website. The line management of CNM is organized into research groups based on capabilities. This adds considerable efficiencies in supporting users because processes, hazards, and tool expertise are organized together and users have multiple staff in a particular capability area to interact with. We emphasize that the thematic research of CNM spans and engages all of the following groups:

- **Nanofabrication and Devices Group**, with Group Leader Anirudha Sumant, specializes in the developing and studying micro- and nanoscale systems to achieve unprecedented control in the fabrication, integration, and manipulation of nanostructures. This includes the incorporation—under cleanroom conditions—of materials and active submicron elements that couple mechanical, optical, and electrical signals to produce working nanofabricated structures.
- **Quantum and Energy Materials Group**, with Group Leader Jeffrey Guest, focuses on the synthesis and fundamental characterization of molecules and materials on nanometer to atomic length scales. This group employs physical deposition and chemical synthesis methods while using a powerful suite of scanning probe capabilities, X-ray probes, transport, and optical measurements—in some cases, simultaneously—to develop next-generation nanostructured materials to address challenges in our thematic research, such as in QIS and clean energy.
- **Nanophotonics and Biofunctional Structures Group**, with Group Leader Richard Schaller, seeks to understand and control light–matter interactions in nanomaterials by studying the dynamics of photo-active processes through time-resolved spectroscopies and microscopies over multiple contrast mechanisms and energy ranges. The group also studies the interaction of light with biological assemblies for nature-inspired research in energy transduction and sensing.
- **Electron and X-ray Microscopy Group**, with Interim Group Leader Jianguo Wen, performs research to achieve local understanding and control of the structure and dynamic behavior of quantum- and energy-related materials at the atomic scale to the nanoscale via advanced electron and X-ray imaging, diffraction, and spectroscopic techniques coupled with data science. Their research bridges the unique capabilities offered by the newly developed UEM and an HXN enabled by the APS-U. The group also drives traditional strengths in high-resolution and in-situ quantitative electron microscopy.
- **Theory and Modeling Group**, with Group Leader Subramanian Sankaranarayanan, works on large-scale molecular dynamics, high-level electronic structure theory, AI/ML quantum and electrodynamics theory, and multi-scale modeling and data-science-based approaches to understand and predict a wide range of phenomena, including nanoscale tribology, microelectronics, thermal and charge transport, and quantum-entangled systems. It also plays a large role in Theme II, AI/ML-Accelerated Analytics and Automation.

A facility the size of CNM also requires dedicated personnel to support science and operations. Approximately one dozen personnel include user program administrators, information technology experts (addressing computer administration, data management, and the development of operations software), safety personnel, administrative professionals, building/facilities management, and senior facility managers (director and deputy director). CNM staffing is rounded out with approximately two to three dozen temporary appointments, which include postdoctoral fellows and visiting graduate students, as well as interns during the summer months.

Overall, CNM's continued success and leadership will depend, in large part, upon: our ability, along with our users, to continue to perform world-class science; investments in differentiating and leading-edge research tools that attract the best scientific users; recruitment and retention of talented scientific staff; and, importantly, our ability to anticipate and influence strategic areas that define future nanomaterials research. Going forward, we will hire research staff in key strategic areas that link to our thematic research in key areas including AI/ML, advanced characterization, and QIS. In addition, as the number of users continues to grow, we will also make new technical staff hires in the most heavily used capabilities that map to our strategic growth areas.

Safety

CNM has responsibility for environment, safety, health, and quality assurance (ESHQ) aspects of operations and, through policies and procedures, defines how responsibilities are delegated from the director through line managers to technically competent staff members supporting user research activities. The CNM program complements Argonne's laboratory-level safety program by incorporating methods, controls, and a work approval approach tailored to the risk characteristics of a user facility and the materials, instruments, and processes that constitute CNM operations. The specifics of the program are periodically updated to ensure compliance with evolving standards, Argonne safety program evolution, and emerging information on hazards. A certified ESH professional is dedicated to helping CNM ensure research productivity and efficient implementation of the applicable ESHQ standards and requirements.

CNM staff collaborate on important ESH projects, such as the Hazardous Gas Response Team. This team developed their activities and formalized them in a guide and job aids, which are maintained by division safety and operations personnel. The guide and aids define appropriate and safe paths assuring prompt and effective control of risks signaled by the facility's toxic gas monitoring system. The team has a balanced combination of safety, operations, and research experience to appropriately respond to gas monitoring system alerts.

CNM takes a precautionary approach when there is uncertainty about the hazard potential of new chemicals, including nanomaterials. This concept guides the hazards analysis and specification of precautions when handling nanomaterials. In this way, CNM contributes to a better understanding and management of ESH concerns associated with nanomaterials and nano-enabled products.

Cybersecurity

CNM's cybersecurity operations are driven by Argonne's cybersecurity posture, which is a required component of the Lab's Authorization to Operate, issued by DOE via the Argonne Site Office. The cybersecurity plan for the Lab is documented in a National Institutes of Standards and Technology–driven framework documented in Argonne's Cyber Office's Cyber Security Program Plan (CSPP), a 375+ page document covering perimeter protection, internal segmentation/separation, network/system monitoring, active response, incident response, configuration management, system management, best practices, auditing/self-assessments, documentation, physical controls, and other topics. CNM implements the CSPP to meet these requirements.

In addition, CNM augments existing policy with additional controls, such as lab system protection using micro-segmentation to provide additional protections for systems that may, due to necessity, deviate from best practices in order to meet the scientific mission. An example would be systems attached to research equipment locked to a particular operating system.

Data Management

CNM recognizes that effective data management has the potential to increase the pace of scientific discovery and promote efficient and effective use of funding and resources. To advance this principle and others defined by the DOE Policy for Digital Research Data Management, CNM has established the following research data management goals:

- Reliably capture and describe scientific data in a way that facilitates preservation and reuse.
- Create quality metadata for data discovery, preservation, and provenance. Our goal is to achieve scalable hosting of data platforms on our Carbon Cluster.
- Design and implement interfaces for users to search for, and interact with, datasets.
- Preserve collected data for long-term users.

Data are stored and curated in compliance with Argonne's data retention policy for scientific research data. This includes the use of granular controls and security measures necessary to keep data safe until it is intended to be shared. CNM also has a data-retention policy for user-generated data, which is described online at "CNM User Information."

5. User Community

CNM strives to attract a broad user community that performs high-caliber, impactful research. Our user community includes researchers from across the country and around the globe. Figure 5-1 displays the makeup of CNM users in FY 2025 as a function of their affiliation. Slightly more than half of our approximately users per year are from U.S. academia, with representation of non-Argonne users from international, industrial, and other government organizations. Figure 5-2 displays the fields of research represented by CNM users.

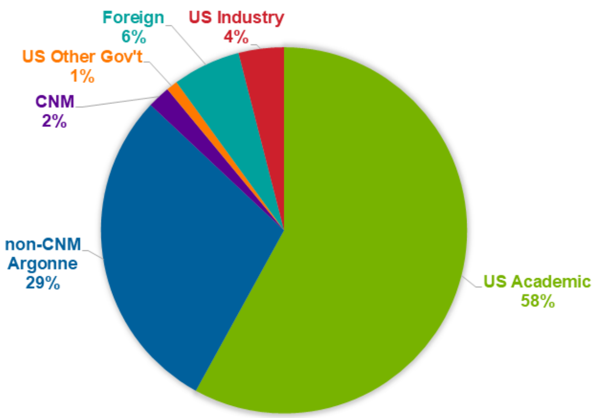


Figure 5-1: *Institutional affiliations of CNM users by affiliation during FY 2025.*

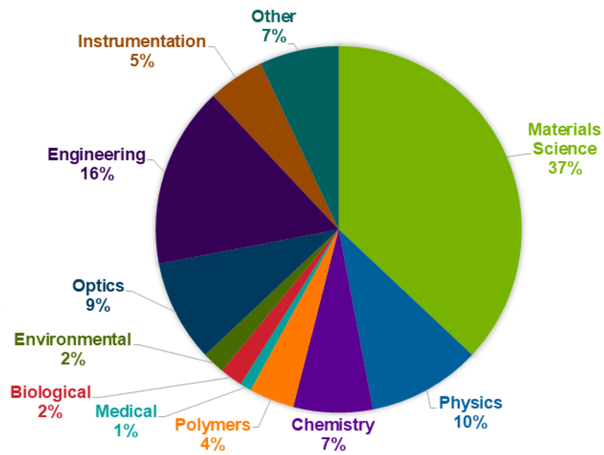


Figure 5-2: *Fields of research identified by CNM users during FY 2025.*

Our users, together with CNM's research/scientific support staff, continue to have an excellent scientific impact, with nearly 300 peer-reviewed publications annually, 57% of which are published in journals with an impact factor above 7 (FY 2025). During FY 2020, the global COVID-19 pandemic impacted our ability to host our usual complement of users. However, demand was still strong, and we accommodated the work of 631 unique users that year. In FY 2020 and FY 2021, we also invested significantly in remote-access capabilities, which enabled users to remotely access more than 30 tools. Due to this effort, CNM began hosting more users in FY 2022 than during the pre-pandemic period. In FY 2025, the number of unique users grew to 1,001, including 706 onsite users and 295 remote users. We continue to plan for a growing remote-access effort, which will be a means to leverage our research impact and reach more users in the coming years. This particularly includes users from institutions that may not have the resources to travel to CNM.

User time is allocated through a proposal submission and review process in which CNM scientific staff, management, and external reviewers all have key roles regarding feasibility, scheduling, and scientific merit. The goal is to operate a process that is fair and equitable based on the scientific and technical quality of the proposals.

Determining a technical strategy that maximizes our impact on science and benefits our users requires us to anticipate future user needs and help shape future areas of focus in the nanosciences. Our future capability and facility upgrades are based on prioritization of science, staffing, infrastructure, and equipment needs. The needs of our scientific themes are a starting point for setting our prioritization directions and are adjusted by accounting for any new initiatives driven by national needs. Discussions with our Scientific Advisory Committee and User Executive Committee, and science strategy discussions during CNM's approximately annual strategic retreat, further inform this prioritization. Emerging areas of research in the nanoscience community are also strongly considered, for example, as defined by national research agency funding directions and strategic documents (e.g., the Office of Science Basic Research Needs Workshops and Roundtables), which indicate future user needs. We also seek feedback from an annual user survey at the end of each proposal project.

CNM is also actively expanding the scope of its science toward future industrial impacts, seeking opportunities beyond its industrial user program. Recently, Mitsubishi Heavy Industries expressed active interest in our superlubricity-related research; the company visited and discussed developing an umbrella CRADA to carry out further research in this area. We also have an active CRADA with Ford Motor company on SEIs in batteries. This work leverages unique facilities including the ALCF, NERSC, and APS, as well as advanced multimodal characterization capabilities within the CNM. Our industry user base is expanding to include user proposals from major corporations such as Meta. We plan to reach out to Chicago's mHUB Innovation Center for Physical Product Development and other regional startup companies including the new Illinois Quantum and Microelectronics Park, a first-of-its-kind campus built for quantum technology and microelectronics innovation and scale-up. CNM is also a part of the Nano-Scale Research Centers for Heterogeneous Integration Platforms (NSR-CHIP). In this microelectronics-focused effort, we plan to work with several semiconductor corporations including Applied Materials, Imec USA, and others. Apart from this, our close research collaboration will continue with Chain Reaction Innovation startups and small regional companies including Creative Microtech, Frore Systems (a Silicon Valley startup), Alcorix, and Iris Light Tech (a spinoff from CNM), memQ, and Caporus Technology.

AI/ML efforts in CNM are expected to positively impact the user experience and enhance the efficiency of user research. CNM scientists are developing tools and methods for faster and more accurate molecular modeling of materials, more efficient interpretation of electron and X-ray microscopy data, and new approaches that combine ML with a physics basis. Exciting new opportunities are also being generated by combining robotics with AI/ML to enable autonomous synthesis and materials processing, providing users with cutting-edge new technologies. Finally, research and development on digital twins will allow users to explore characterization experiments and conditions before arrival at CNM, enabling users to jumpstart their visit and efficiently target the experiments most likely to succeed.

Appendix 1: Major CNM Capabilities

CNM maintains a large suite of capabilities, while regularly upgrading or procuring new capabilities. We maintain a full list of capabilities on our "Tools & Capabilities" page. This appendix provides detailed descriptions of major CNM capabilities that have been developed by our staff, where additional details are warranted to aid users.

Quantum Information Science (QIS) Capabilities

For the past several years, CNM has added several new tools focusing on QIS research, dramatically impacting our activities within Theme I, Quantum Coherence by Design. CNM is the first user facility among the NSRCs that offers comprehensive capabilities for studying coherent interactions in solid-state optical and spin-based qubits for QIS. Examples of the new tools and capabilities follow.

Ultra-low-temperature, dilution-refrigerator-based experimental systems are essential to conducting QIS research but are expensive and thus beyond the reach of many users. To attract a broad range of users and collaborators, CNM set up a new low-temperature laboratory dedicated to research covering most qubit platforms—from superconductor to semiconductor qubits and defect centers to single electrons. This laboratory opened to users in September 2019. The system is equipped with microwave spectroscopy capabilities for spin-based studies, and soon, a femtosecond ultrafast laser system will be integrated with the dilution refrigerator system. A second tool, the adiabatic demagnetization refrigerator (ADR), became available to users in the October 2021 user proposal call. The ADR offers faster cooldown times than a dilution refrigerator, with a slightly higher base temperature of 30 mK. It is also equipped with microwave spectroscopy capabilities for studying spin excitations in nanomaterials. Collectively, these systems will enable studying ultrafast quantum dynamics, single-molecule imaging and sensing, and collective spin waves (magnons), and conducting QIS research on single-atom/molecule electron spin.

We have also developed strong quantum entanglement and transduction (QET) capabilities. These are a comprehensive suite of user tools being developed for the study of quantum optics and hybrid quantum networks linking photons, spins, and magnons. QET capabilities will enable single-photon correlation spectroscopy, magneto-optical spectroscopy, optically detected magnetic resonance spectroscopy, magneto-electrical spectroscopy covering microwave and optical frequencies, and new QIS computational modeling environments. A photon correlation microscope is available for users, enabling time-gated photon correlation (and a 9 Tesla magnet equipped with a microscope cryostat) for magnetic field studies of spin-dependent energy levels. The instrument has continuous-wave and femtosecond pulsed lasers covering wavelengths from 370 to 1,300 nm, as well as visible and near-IR cameras and photon-counting detectors for imaging. It can be used to conduct static and time-resolved spectroscopic studies under external magnetic fields. Our theory and modeling capabilities in QIS play a key role in informing and advancing our experimental capabilities. We model the effects of dissipation and noise via quantum master equation approaches, use ML to accelerate quantum measurements, and develop quantum algorithms for materials modeling.

Finally, as described in Theme I, Quantum Coherence by Design, we added major multimodal tools for QIS that are now available to users, including the QuEEN-M and AQuISS. As described in that section, additional HXN capabilities were added to the APS-U, enabling enhanced optical characterization of defect emission, correlated with detailed structural information only achievable at the synchrotron.

Ultrafast Electron Microscopy (UEM) Laboratory

The UEM was installed in the spring of 2019 and began full user operations in 2021 as the first user tool for UEM within the NSRCs. In its final form, this tool allows users to access time-resolved stroboscopic imaging, diffraction, and spectroscopy/spectral imaging capabilities, built using a combination of commercial vendors for TEMs, lasers, detectors, and column integration. The system enables researchers to observe dynamic reversible processes in events that are optically triggered via laser excitation at wavelengths selectable over a wide range from 325 to 2,000 nm, and it is being further developed for electrical and mechanical triggering of complex material phenomena. These capabilities will be significantly enhanced over the next three years through a unique correlative integration of ultrafast electron and X-ray microscopy coupled with ML approaches for multimodal multi-platform data synthesis.

Artificial Intelligence (AI) for Materials Science Capabilities

CNM has set forth a comprehensive software and hardware upgrade plan that leverages recent advances in AI to accelerate our computational materials science capabilities. The upgrades include developing user-friendly capabilities and the ability to process large volumes of data effectively. Many of these are described in Theme II, AI/ML-Accelerated Analytics and Automation. More details are given below.

Fully Automated Nanoscale to Atomistic Structure from Theory and eXperiment (FANTASTX)

We developed a computer vision-based software tool that enables near-real-time interpretation of images generated from electron and scanning probe microscopies. FANTASTX ingests experimental images as input and makes comparisons with thousands of atomistically simulated crystallographic or morphological structures to identify an “optimally matched structure” in a manner analogous to facial recognition software. The optimization is carried out using genetic algorithms, where the cost function includes both the degree of match as well as minimization of the energy of the configurations.

Bridging Length/Time Scales via Atomistic Simulation Toolkit (BLAST)

Molecular modeling is a powerful tool today. Historically, however, a gulf existed between the handful of research groups that develop new interatomic potential models for materials modeling (often involving several years of effort) and the increasingly large user community that applies these models. At present, users do not generally have the flexibility to adapt these predefined potential models to problems that interest them. BLAST, a computational workflow tool, overcomes this barrier by allowing users to create their own models. It provides a simplified framework that permits users to handle various types of training data, optimize potential functions using evolutionary algorithms, and cross-validate their model predictions. BLAST users can select functional forms available in popular molecular dynamics codes, as well as apply combinations of global and local optimization schemes to generate force fields for molecular simulations. Such a general-purpose tool holds promise for identifying structure-property-processing relationships in various material classes.

Carbon Cluster

CNM is investing strongly in our Carbon Computer Cluster to handle all problems associated with experimental data analysis and theoretical modeling, with additional capabilities for handling AI problems. The Carbon Computer Cluster currently has 130 nodes, 4800 Xeon cores, and 48 graphics-processing-unit-oriented nodes, each with two data-center-class GPUs, all connected over a high-speed InfiniBand interconnect. The Carbon Computer Cluster has 500 TB of storage (Lustre). We are planning a major upgrade to the Carbon Computer Cluster in FY 2026 to continue to enhance this tool. It is currently the most accessed user tool in CNM and produces the most publications per year relative to any other capability in CNM.

Superlubricity Science Laboratory

For several years, CNM scientists have explored and demonstrated the remarkable result of true superlubricity (near zero friction) at the macroscale using nanoscroll-shaped solid lubricants of diamond nanoparticles wrapped with graphene. This work continues to grow and expand to other materials systems via partnerships with two major industry leaders through two DOE Technology Commercialization Fund awards that CNM received. Given CNM's leadership in this space, we are continuing to grow our capabilities in superlubricity science at the nanoscale.

A Superlubricity Science Laboratory was recently configured to include a multifunctional tribometer with integrated confocal microscopy and Raman spectroscopy. We added new capabilities that will allow us to carry out in-situ TEM of tribological interfaces and changes upon loading and assess the wear/friction behavior of 2D materials and nanomaterials at elevated temperatures (~500°C), uncovering the detailed wear/friction behaviors of these materials that are unknown today. Combining these new and unique capabilities will enable our user community and our own researchers to understand and study nanomechanical and wear/friction behaviors under realistic conditions and across the entire length scales of relevance (nanometer to microns) for the first time.

Cleanroom Facility

In 2017, using ~$9 million in funding from Argonne, the CNM cleanroom expanded from 12,000 ft^2 to ~18,000 ft^2. CNM users have full access to the expanded portion of the cleanroom. Going forward, in agreement with Argonne management, the additional space will be used to house both CNM and non-CNM tools, and CNM will be responsible for managing this space. This expansion solved our space crunch for cleanroom tools, and the extra square footage enables our planned modernization of the nanofabrication facilities. Several new tools and upgrades have been added in the CNM cleanroom, including a FastScan AFM for metrology, replacement of a critical point dryer for micro-electromechanical systems release, a thermal evaporation system from Angstrom, a second maskless aligner, a new carbon vapor deposition tool for microelectronics studies, a PFIB tool for reducing contamination of materials frequently encountered with the more common gallium ion FIB, a field-emission scanning electron microscope, and many others.