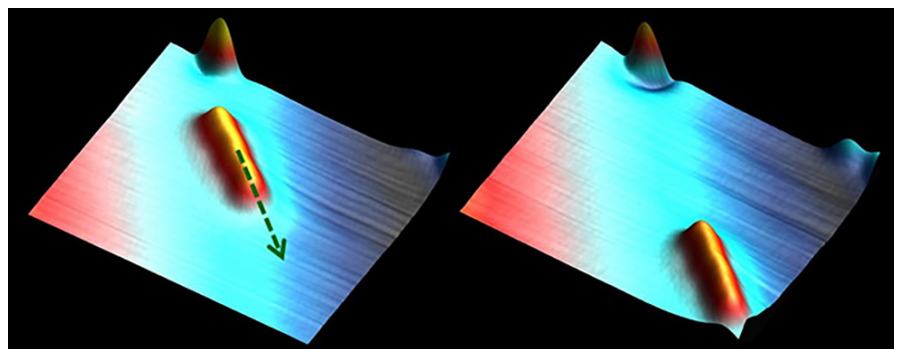
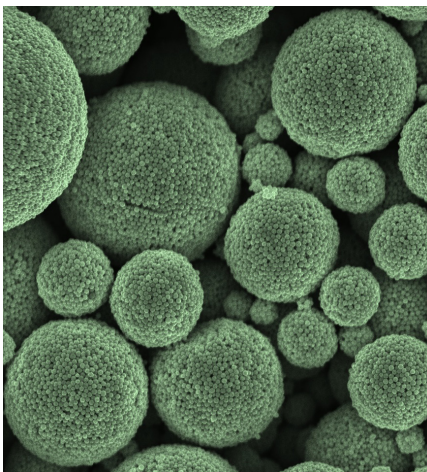
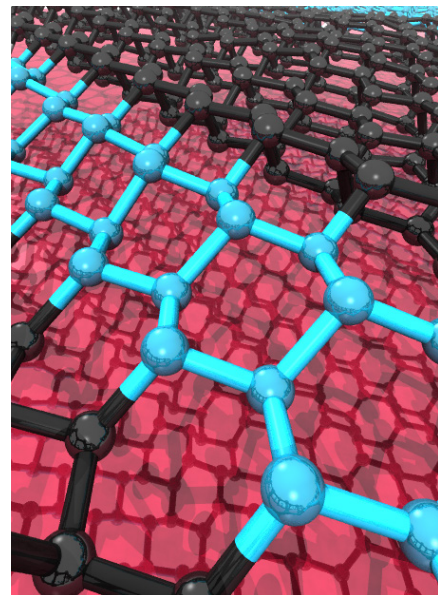
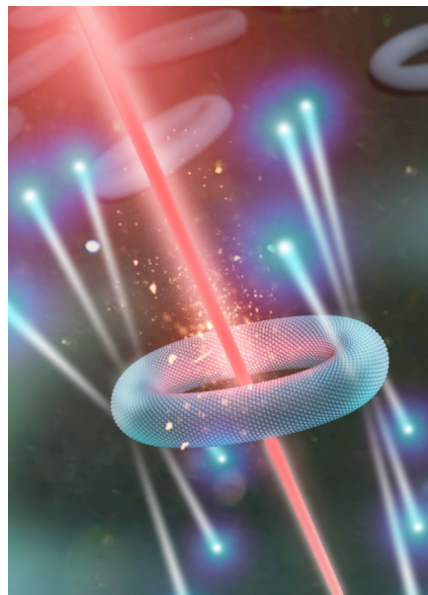
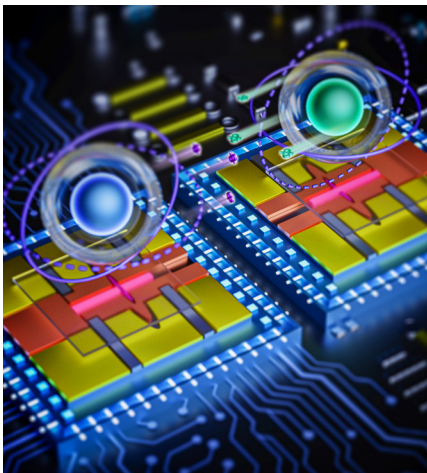


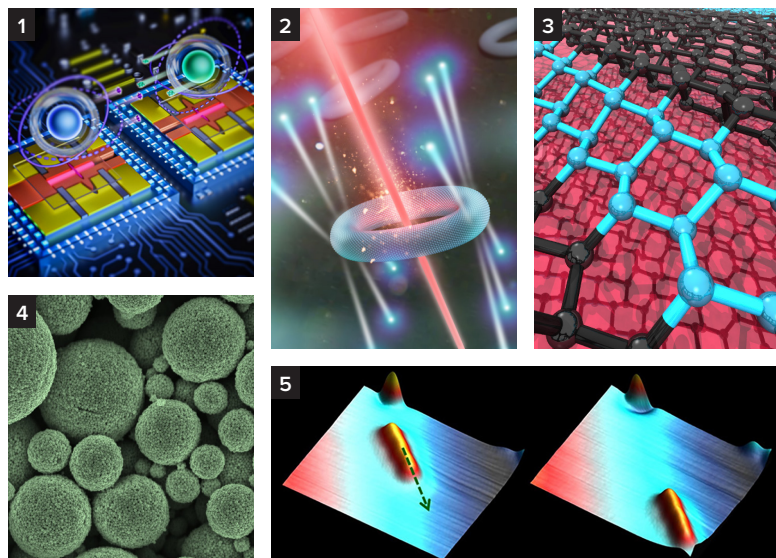
CENTER FOR NANOSCALE MATERIALS

STRATEGIC PLAN

Fiscal Year 2024



ON THE COVER



1. Illustrated are two single electron qubits (blue and green balls) on solid neon (transparent square slabs on top of the circuit chip) with ultralong coherence time, strongly coupled with a common superconducting microwave resonator (red circuit lines). (Nature Physics **20**, 116 [2024]) <https://www.nature.com/articles/s41567-023-02247-5>
2. Depiction of a cadmium selenide quantum ring emitting light in one axis. Optical transition dipole moments measured with angle-resolved photoluminescence spectroscopy and high-order scanning laser microscopy, conducted in part at CNM. Empirical tight-binding calculations of the wave functions also performed in part at CNM. (Nature Commun. **10**, 3253 [2019]) <https://www.nature.com/articles/s41467-019-11225-6>
3. The strain-induced structural phase transformation of black to blue phosphorene using machine learning models is illustrated. (J. Phys. Chem. Lett. **13**, 1636 [2022]) <https://pubs.acs.org/toc/jpclcd/13/7>
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://onlinelibrary.wiley.com/doi/full/10.1002/ange.201813963>
5. Scanning Tunneling Microscopy images before and after manipulation of Sexiphenyl (6P) molecule on Ag(111) surface revealing anisotropy due to the shape and interaction of 6P molecule on Ag(111) surface. (Nano Letters **21**, 6391-6397 [2021]) <https://doi.org/10.1021/acs.nanolett.0c04974>

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Table of Contents

Acronyms	ii
1. Introduction and Overview	1
2. Science and Technology	4
Theme I—Quantum Coherence by Design	4
Theme II—AI/ML-Accelerated Analytics and Automation	6
Theme III—Ultrafast Dynamics and Non-Equilibrium Processes	8
Theme IV—Interfaces, Assembly, and Fabrication for Emergent Properties	11
Theme V—Nanoscale Discovery for a Sustainable Energy Future	13
3. Capabilities	15
4. Operations	16
Staffing	16
Safety	17
Cybersecurity	17
Data Management	18
5. User Community	19
Appendix 1.a: Major CNM Capabilities	21
Appendix 1.b: Future Capability Enhancements at the CNM	24
Appendix 2: Diversity, Equity, Inclusion and Accessibility at the CNM	27

Acronyms

2D	two dimensional
3D	three dimensional
ADR	adiabatic demagnetization refrigerator
AFM	atomic force microscopy
AI/ML	artificial intelligence/machine learning
ALCF	Argonne Leadership Computing Facility
APS	Advanced Photon Source
APS-U	Advanced Photon Source-Upgrade
AQuISS	Atomic Quantum Information Surface Science
BLAST	Bridging Length/timescale <i>via</i> Atomistic Simulation Toolkit
CASTING	Continuous Action Space Tree search for INverse design tool
CL	cathodoluminescence
CNM	Center for Nanoscale Materials
CSPP	Cyber Security Program Plan
DEIA	diversity, equity, inclusion, and accessibility
DFT	density functional theory
DOE	Department of Energy
DR	dilution refrigerator
DAC-STEM	double-aberration corrected scanning transmission electron microscope
ESHQ	environment, safety, health, and quality assurance
FANTASTX	Fully Automated Nanoscale To Atomistic Structures from Theory and eXperiment toolkit
GUI	graphical user interface
HPC	high-performance computing
HXN	Hard X-ray Nanoprobe
MIE	major items of equipment
NSRC	Nanoscale Science Research Center
NST	Nanoscience and Technology
PIER	Promoting Inclusive and Equitable Research
PL	photoluminescence

QET	quantum entanglement and transduction
QIS	quantum information science
QuEEN-M	Quantum Emitter Electron Nanomaterial Microscope
SPP	surface plasmon polariton
STEM	scanning transmission electron microscope
STM	scanning tunneling microscopy
TEM	transmission electron microscopy
TPCS	transient photoelectron and cathodoluminescence spectroscopy
UEM	ultrafast electron microscopy
UHV	ultrahigh vacuum
UOM	ultrafast optical microscopy
XEOL	X-ray excited optical luminescence

1. Introduction and Overview

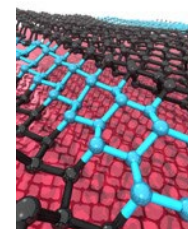
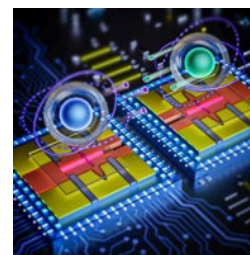
Our vision for the Center for Nanoscale Materials (CNM) at Argonne National Laboratory is to continue to enhance its role as a world-leading research center in nanoscience, while serving and leveraging a large user science community to produce basic science discoveries that impact the needs and critical technologies of the United States. These include, for example, discoveries that impact clean energy, quantum information science (QIS), artificial intelligence/machine learning (AI/ML), optoelectronics and microelectronics. 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.



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.

Our research is organized into five cross-cutting scientific themes. The themes provide a framework for our scientific strategies, which align with national science priorities. Brief summaries of each of the CNM themes are given below:

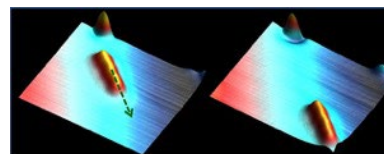
- I. **Quantum Coherence by Design.** The goal of this theme is to harness CNM’s expertise and capabilities in nanoscale synthesis, fabrication, characterization, and theory to discover fundamental mechanisms, novel materials, and innovative system designs for transformative insight and impact in QIS. 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.** In this theme, our work focuses on the development and use of AI and ML to enable multiscale simulations and real-time imaging, perform information extraction from multimodal X-ray and microscopy characterization, and enable autonomous synthesis and processing of materials beyond equilibrium. This theme also includes research on “digital twins,” which allows users to explore characterization experiments and conditions before arrival at the CNM, enabling users to efficiently target the experiments most likely to succeed.



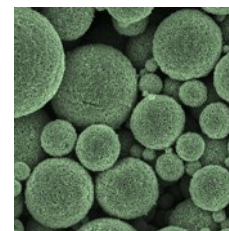
III. **Ultrafast Dynamics and Non-equilibrium Processes.** The goal of this theme is to study and control energy flow and structural changes in nanoscale materials on femtosecond to second timescales over angstrom to macroscopic length scales in order to discover new uses and improve device efficiencies of nanostructured systems. This theme leverages the 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.** In this theme we focus on the emergence of new properties from interfaces, assembly, and fabrication. The creation of emergent properties refers to behaviors that arise from materials interacting in interfaces, or through assembly and fabrication, that are not predictable from 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 a Sustainable Energy Future.** The goal of this theme is to utilize the CNM's expertise in computational modeling, synthesis, and advanced characterization to accelerate the discovery, research, and development of nanoscale platforms for a clean and sustainable energy future. Research topics include, for example, batteries, solar power, photocatalysis, electrocatalysis, and carbon capture/reduction to impact energy storage, conversion and the circular economy.



The CNM employs unique expertise and capabilities to maximize the impact of our research efforts. This enables cross-cutting and collaborative efforts across the Center in support of thematic research. Three examples follow. The first example is our effort to develop and apply AI/ML for a large range of studies and applications that leverage the exceptional Argonne-wide high-performance computing (HPC) facilities. Efforts include AI/ML for rapid materials discovery and for information extraction and analysis of experimental datasets. In these efforts, CNM scientists are developing (i) tools and methods to scan through synthetic and preparatory conditions faster, (ii) more accurate molecular modeling of materials and on-the-fly interpretation of electron and X-ray microscopy data, and (iii) autonomous synthesis/processing of nanoscale materials, including those that can contribute to easily processed microelectronics applications, as well as polymer materials that can potentially be recycled more easily as part of a circular economy. Our AI/ML efforts thus impact other themes in many ways, such as predicting new compounds for solar energy conversion or energy storage, or autonomously synthesizing or processing materials of interest for microelectronics.

A second example is our cutting-edge ultrafast electron microscopy (UEM) capability. We have already started growing a new user base in nanoscale dynamics by being the first Nanoscale Science Research Center (NSRC) to offer user capabilities (available as a general user tool in March 2021) for UEM. This tool, which we carefully designed, opens the door for a specialized technique that has to date been available only to a few research groups that specialize in technique development. The UEM represents a key experimental method that can offer insights to ultrafast (sub-picosecond) structural and chemical change to a wide range of materials systems with diversified potential applications, including understanding heat transfer through materials important for QIS and microelectronics.

A third example is in materials for quantum information, in which we have been investing since 2016. At this juncture, major user capabilities include ultralow temperature cryostats equipped with microwave spectroscopies, two electron paramagnetic resonance spectroscopy tools, and extensive quantum optical microscopy tools. We are also working to bring two additional major QIS tools to users in FY 2024. The

first tool is 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. The second tool is the Quantum Emitter Electron Nanomaterial Microscope (QuEEN-M). QuEEN-M is 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.

Research at CNM is closely tied to significant capabilities at the Advanced Photon Source (APS) and the Argonne Leadership Computing Facility (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. Furthermore, researchers at CNM work closely with staff in many Argonne divisions across Argonne Directorates.

In this Strategic Plan, we provide an outline of our science and technology research plans. This will be followed by a description of our operations and strategic directions for enhancement, including in safety, cybersecurity, data management, and staffing. We close with a description of our user community and strategic plans for diversity, equity, and inclusion for our users and staff.

2. Science and Technology

As introduced above, 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 Non-Equilibrium Processes, (iv) Interfaces, Assembly and Fabrication for Emergent Properties, and (iv) Nanoscale Discovery for a Sustainable Energy Future. 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.

We describe here our specific strategic plans for each of the five themes. It is not our intent to comprehensively list all the projects that could be carried out within CNM, but rather to focus on broader research directions within the five themes. Each theme has three thrusts that provide the 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 focus on leveraging the unprecedented characterization and control that have been achieved through modern nanoscience to develop a deeper understanding and new experimental platforms for QIS. Our approach to QIS research and the development of capabilities involves three thrusts: *Next Generation Quantum Systems*, *Control of Coherence*, and *Quantum Transduction*.

The *Next Generation Quantum Systems* 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 in nature, and their development will benefit immensely from the 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 of research in this thrust, 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) and reported the initial discovery in a journal article (*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-electron qubit platform takes

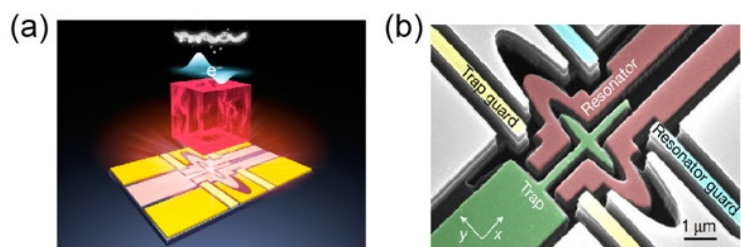


Figure 2-1: (a) Schematic of a single-electron qubit trapped on a solid neon surface and interacting with a superconducting coplanar stripline resonator. (b) Scanning electron microscopy image of the device around the electron trap and photon coupling region. Future work will target continued improvement of quantum coherence properties and entanglement to further enable QIS applications (*Nature* **605**, 46 [2022]).

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. Recently, we have further improved the qubit performance, reaching a record long coherence time of the electron qubits, with T_1 and T_2 reaching the 100 μs scale (*Nature Phys.* **20**, 116 [2023]). This is greater than any existing semiconducting or superconducting charge qubit. High-fidelity single-qubit gates and high-fidelity single-shot readout were also demonstrated. Importantly, we further demonstrated the simultaneous

strong coupling of two qubits with a common resonator, which is an important step towards qubit entanglement and two-qubit gates.

Within this thrust, we are developing newly commissioned tools awarded by DOE for QIS research that enable deterministic placement and detailed characterization of defect qubits of interest for quantum optics. Given that 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, such as deterministic emission and controlled coherence. Our QuEEN-M platform, which 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. It further enables the investigation of optically active defects and dopants with unprecedented spatial resolution, as well as photodynamic studies, with the goal of revealing the complete picture of the electronic structures of quantum emitters by nanoscale CL correlative microscopy and time-resolved CL for lifetime and coherence measurements beyond the optical diffraction limit. Due to the difficulty of imaging buried quantum emitters embedded in three-dimensional (3D) materials, atomically thin or few-layer two-dimensional (2D) materials will enable nanoscale CL correlative microscopy with atomic-resolution STEM.

Progressing beyond characterization, the *in-situ* formation, processing, and measurement of quantum emitters will be studied using the QuEEN-M. 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), although this is still an uncontrolled process under most circumstances. Other samples (e.g., freestanding diamond membranes) will be studied for deterministic placement of nitrogen vacancy centers in diamond.

This leads to the second thrust, *Control of Coherence*, which addresses the fact that 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. Additional challenges relate to the fact that solid-state spin qubit research has traditionally centered on defects or dopants in highly environmentally controlled environments or buried deep inside near-perfect crystals, significantly curtailing their potential utility and limiting the ability to control and place these systems with precision. We are addressing this challenge through the development of the AQuISS lab, awarded by DOE for QIS research. Through this lab, we plan to open a new frontier in nanometer-scale control over *optically active spin quantum systems* by combining quantum control (both microwave and optical) and advanced techniques of surface science, including characterization and manipulation with scanning probe microscopy, on controllable ultrahigh vacuum (UHV) surfaces. In addition to near-surface bulk defects, we envision many promising new systems can also be developed *at* surfaces, including surface defects, dopants, molecules, and engineered van der Waals materials.

We emphasize that both the QuEEN-M and AQuISS laboratories will bring highly advanced and unique capabilities in QIS to the CNM user communities. And we are not stopping there. We are also leveraging our strong collaboration with the APS to develop complementary nano-focused hard X-ray microscopy capabilities that will provide a unique opportunity to understand the quantum response of defects. Using CNM's unique Hard X-ray Nanoprobe (HXN) capability at the APS, we recently developed a technique of 3D Bragg projection ptychography. Building upon promising results already obtained in showing how sound (using surface acoustic waves) can modulate a SiC defect qubit (*Nature Phys.* **15**, 490 [2019]), we intend to use this technique extensively to visualize near-defect strain directly in quantum materials in the coming years. We are also planning the development of nano-focused X-ray excited optical luminescence detection and spectroscopy at the HXN enabled by the 100x coherent flux increase of the near-term APS-Upgrade project (currently planned to be completed in late FY 2024). With this capability, data will be collected simultaneously with diffraction-based Bragg ptychography and used both to locate

optically active atomic defects to within ~10-nm precision within 3D strain images of crystalline volumes and to provide an *in-situ* spectroscopic view of the defect-level response to the local structure.

In the final thrust, *Quantum Transduction*, 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 of interest in QIS. We plan to leverage our recent research on piezo-optomechanical transducers (*Nat. Commun.* **11**, 3237 [2020]; *Optica* **8**, 1050 [2021]), as well as the development of various qubit systems at CNM, to demonstrate and study quantum transduction. We specifically plan to connect multiple CNM laboratories with QIS research via fiber-optical quantum channels to demonstrate novel capabilities of remote quantum state and information transfer. The qubits will be of different varieties (such as quantum optical and charge-based qubits). This work will be supported by strong theory efforts in evolving, high-dimensional quantum states. Quantities to estimate or measure are time-dependent correlation functions, including out-of-time-order correlators, measures of fidelity and distance between different density matrices, and quantum Fisher information. These tools will allow users, for example, to manipulate and interconnect microwave and optical qubits to enable experimental research on new devices. Theory and simulation are essential both to enable the experimental QIS outlined in this plan and drive new experiments and directions. We will also take advantage of machine learning to accelerate challenging quantum science measurements.

Theme II—AI/ML-Accelerated Analytics and Automation

Our strategic plans in this theme center on utilizing recent AI/ML and HPC advancements for data analytics to rapidly advance materials discovery and greatly enhance information extraction from a wide range of experimental characterization experiments. We plan to develop transformative theory and theory-experiment capabilities, while bringing them to the research community in user-friendly platforms. This work leverages major computing capabilities in the CNM and at Argonne, as well as computational user facilities across the DOE complex. The theme's research plan can be summarized by three thrust areas: *Multi-fidelity Scale Bridging and Materials Design*, *Theory Guided Information Extraction from Experimental Characterization*, and *Autonomous Synthesis of Nanoscale and Metastable Materials*.

The *Multi-fidelity Scale Bridging and Materials Design* thrust focuses on using our diverse modeling and simulation expertise to bridge the gap between the accuracy and efficiency of the various simulation models. This involves utilizing AI/ML algorithms to address spatiotemporal challenges in molecular and mesoscopic simulations. Our research plans involve developing machine learning 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/timescale via Atomistic Simulation Toolkit (BLAST - *MRS Advances* **6**, 21 [2021]), the Continuous Action Space Tree search for INverse design tool (CASTING - *npj Computational Materials* **9**, 177 [2023]), and the Fully Automated Nanoscale To Atomistic Structures from Theory and eXperiment toolkit (FANTASTX – *Microsc. Microanal.* **24**, 510 [2018]). New features and optimization modules will be implemented to broaden their functionalities. Special attention will be given to refining the graphical user interface, ensuring user-friendliness for non-experts. Our focus extends to simplifying the handling and importing of datasets, easing design and discovery tasks for novice users.

We are applying ML approaches to materials discovery in technologically important materials. An example of our work is to combine ML with first-principles computational modeling, such as with density functional theory (DFT), in a way that accelerates 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, and quantum applications. Thus,

ML combined with DFT can impact important fields such as photovoltaics and optoelectronics. Here, native and non-native point defects control carrier concentrations and lifetimes, while extended defects, such as 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 quantum information science applications, where the thermodynamics and charge and spin properties of defect complexes are crucial for next-generation defect qubits. This strongly connects to the Quantum Coherence by Design theme and is one example of how our themes complement and enhance the other themes of the center.

The power of combining ML with first principles modeling can be demonstrated by attempts to understand the impact that grain boundaries and dislocation cores play in controlling power conversion efficiency in thin film photovoltaic materials, such as CdTe. Passivation of grain boundaries reduces recombination, but the choice of stable, effective passivants is challenging. Using realistic dislocation core structures obtained from STEM, we have identified different passivants/co-passivants and performed DFT calculations to understand their properties (*Solar Ener. Mater. Solar Cells* **232**, 111279 [2021]). By understanding the origin of the midgap states in different dislocation cores due to DFT analysis, we plan to impact the design of appropriate passivants and co-passivants to optimize performance. In a second example, the approach is further extended to perovskite halides both for improvement of defect properties (*J. Mater. Sci.* **57**, 10736 [2022]) and for the design of perovskite halide (ABX₃) materials with different A and B site cations that are promising for photovoltaic applications. In general, DFT+ML computations are a promising pathway towards materials design that we plan to leverage in the coming years.

In the second thrust of *Theory Guided Information Extraction from Experimental Characterization*, we seek to speed information extraction from multimodal experimental datasets, expediting scientific discovery and utilizing them for dynamical simulations or as training data to enhance models. This is an increasingly important need as experimental tools grow in complexity and the amount of information produced.

A recent example of our progress in information extraction is the development of a tool that automates the fusing of atomic-scale image simulations into experiments. Such experiments involve scanning transmission electron microscopy (STEM) and scanning tunneling microscopy (STM). While “simulation-to-experiment” comparisons can link information about mechanisms generating an experimental observation to parameters and/or specific structures used in a simulation, this requires a 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. It enables the “fusion” of atomic-resolution materials imaging simulations into the experimental images to which they correspond (*Small* **18**, 2102960 [2022]). Ingrained has been demonstrated for several cases, including the grain boundaries of CdTe, the surface of pristine Cu₂O, and the surface of a 2D borophene (hydrogenated borophene). We expect that both computational researchers and microscopists will find practical use cases to add to these examples.

Innovation in advanced characterization tools that produce large datasets serves to drive our future plans in this thrust. Scientific user facilities are developing unique and complex tools with high data production. Locally, the CNM’s Ultrafast Electron Microscope (UEM) and the CNM/APS’s HXN tool, which is capable of coherent diffraction imaging, serve to underscore the need for more efficient information extraction. Our approach going forward involves developing AI/ML algorithms and workflows for swift analysis of 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 knowledge discovery. Making these capabilities available in a user-friendly framework or application is always a focus of our work in this area.

For the third thrust area, *Autonomous Synthesis of Nanoscale and Metastable Materials*, we aim to establish an AI-guided infrastructure empowering users to autonomously control metastability across diverse length scales—from single atoms to nanoscopic domains and mesoscale morphology (*Chem. Mater.* **35**, 3046 [2022]). We seek to develop a state-of-the-art experimental paradigm based on a modular robotic system driven by AI/ML-based methods. The goal is to efficiently search large, complex parameter spaces for emerging classes of nanomaterials discovery. As an example, we are developing “PolyBot,” a ML-integrated modular robotic material discovery platform. This autonomous synthesis platform includes advanced synthesis, processing, and characterization capabilities, as well as an AI/ML method embedded software package. We have already demonstrated a closed-loop optimization of highly conductive polymer nano films via autonomously turning formulation and processing conditions.

In the next five years, we will continue to upgrade the capabilities of this autonomous synthesis platform with more experimental functionalities (e.g., synthesis capabilities and analysis tools) and AI/ML methods for different staff and user projects. More importantly, we will use this newly developed platform to accelerate the discovery of electronic functional polymers for eco-friendly electronics, peptides with desired sequences, and inorganic nanoparticles with desired properties. An example of one

direction that we expect to be fruitful in the coming years is the development of robust and stretchable polymeric materials to be used as sensors for medical diagnostics and other applications (Figure 2-2).

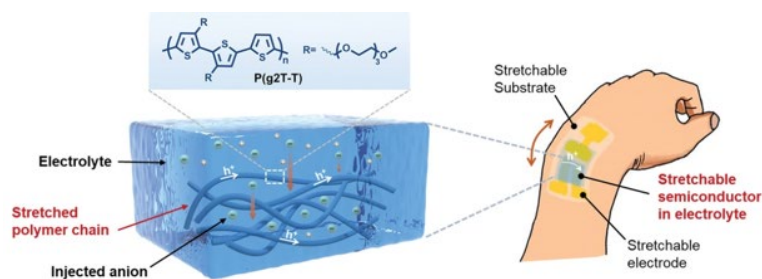


Figure 2-2: Schematic of the mixed ion and hole transport within a functionalized polythiophene film, to be developed for medical diagnostics applications (*Adv. Mater.* **34**, 2201178 [2022]). We are targeting autonomous synthesis and processing of polymer films for a range of additional impacts (including clean energy, microelectronics, and the circular economy) over the next five years.

Theme III—Ultrafast Dynamics and Non-Equilibrium Processes

Today, there is significant need for interrogating, visualizing, and understanding time-dependent phenomena in materials at the nanoscale. This includes understanding energy flow and loss in energy conversion materials, evolution of metastable materials and lattice phase changes, non-equilibrium mechanical responses, plasmonic processes, and the dynamics of the interaction of materials with various excitation quanta (such as optical, magnetic, or electronic) on such time scales. Constrained by the capability of experimental equipment, our window into this world has been limited so far. However, recent advancements in instrumentation are enabling us to change this by probing new contrast mechanisms at greater spectral ranges with high temporal resolution. We are investing extensively in tools for dynamical studies. In fact, we currently have spatiotemporal tools that can span 15 orders of magnitude in time and six orders of magnitude in space at high sensitivity. In the next five years, we aim to offer new tools, methods, and approaches to target central problems in condensed matter physics, novel optical phenomena, and chemical processes, with impact 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*.

Our plans in the *Optical and Carrier Dynamics in Nanomaterials* thrust center on the fact that many potential technologies rely on control of a material’s optical properties and electrical charges to achieve a particular functionality, such as energy conversion, optical switching, or lasing. We believe that nanoscience has a strong role to play here, because nanostructuring makes available an additional toolset to control optoelectronic properties that are impacted by the size, shape, and composition of a

nanomaterial. Our research plans extend to discovery of new electronic states in quantum confined semiconductors, hybridization of plasmonic transitions in nanomaterials, and efforts to achieve efficient charge and energy transfers.

As an example, we are and will continue to study the rich chemistry and physics of colloidal semiconductor quantum wells, which serve as versatile colloidal analogs to epitaxial quantum wells. We have mastered their synthesis and developed chemical methods to tune their electronic structure (*Chem. Mater.* **32**, 5916 [2020]), as well as characterized them for their relaxation times (*ACS Nano* **14**, 12082 [2020]) and dynamic hot electron properties (*Nanoscale* **14**, 1340 [2022]). We have also found that colloidal nanoplatelets have narrow, thickness-dependent intraband absorptions that reside in the near-infrared regime (Figure 2-3). The tunability is remarkable when compared to

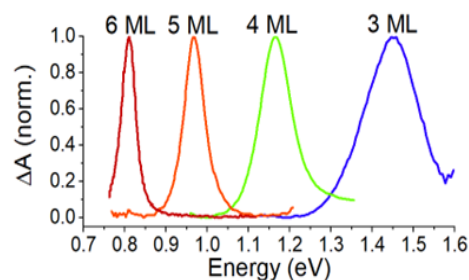


Figure 2-3: Tunable intraband transitions of CdSe colloidal quantum wells, which span a wide range of near-infrared spectrum.

typical epitaxial systems, and colloidal systems will likely be able to be synthesized at scale. We plan to continue exploring the dynamics of these materials, with functionalities for ultrafast optical switching (described in U.S. Patent No. 11,333,908), as well as additional optical technologies. We expect this to be a very active area of research for the next several years in the CNM. In this thrust, we plan to further explore the dependence of the dynamics of nanomaterials on environmental conditions, including the self-assembly of nanoparticles into larger structures and the dependence of optical properties on collective processes such as phonons. We also plan to 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]) and is cooperative with the Quantum Coherence by Design theme.

In the *Engineered and Responsive Dynamics of Strain and Mechanical Motion* thrust, we seek to understand and predict the behavior of mechanical structures as their dimensions are reduced to the nanoscale. For example, it is known that strain can be of growing importance in determining mechanical behavior in a nanostructure as compared to the bulk material. This presents the possibility of new functional properties that depend on building an understanding of dynamically driven nanostructures. We plan for joint theoretical and experimental efforts, where our multi-scale materials modeling expertise and inverse design, combined with extensive and sensitive dynamical characterization tools, will be able to discern mechanical behavior down to the nanoscale. This will impact the connections between light-matter interactions and phonons. The impact of interacting nanomechanical oscillators on optical response, or of mode-coupled nanomechanical oscillators, will be explored.

This leads to the third thrust, *Dynamics of Ordering and Response of Hierarchical Assemblies*. We plan to probe structural evolutions in non-equilibrium nanoscale systems, as well as to produce and characterize dynamics influenced by assembly and/or ordering of nanoscale materials. Examples include systems driven out of equilibrium by external fields, through chemical potential, or near phase transitions. We further plan to combine real- and reciprocal-space imaging techniques with molecular dynamics simulations and AI-driven data processing to understand how these system evolve and to correlate structural and dynamical information with the physical properties of the system to achieve advanced functionality. We plan to explore such phenomena in varied materials, including, for example, biomimetic peptide assemblies, self-assembled colloids, and complex fluids. In many of these cases, probing these non-equilibrium processes requires an *in situ* probe that is capable of measuring structure and dynamics simultaneously. To address this, we developed a rheometer setup for small angle X-ray scattering to study the oscillatory shear on a highly monodispersed silica nanoparticle colloid at different strain amplitudes (*J. Phys. Chem. B* **127**, 7408 [2023]). This is another example of our collaborations with the APS and leveraging of DOE user facilities to provide unique capabilities to our users in the coming years.

In support of these thrusts, we are continually updating 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, infrared photons for vibrational modes, THz photons for transient conductivity, or X-ray photons for structural dynamics. Additionally, we seek to improve our ability in the optical regime to provide spatial resolution with dynamical capabilities. This will complement the dynamical capabilities currently present, but which we plan to develop further for electrons and X-rays via, respectively, the UEM and HXN that were introduced earlier. The plans for optical, electron, and X-ray dynamics are described below.

Our research in ultrafast optical physics will expand into ultrafast optical microscopy (UOM) and newly offered 2D transient terahertz spectroscopy. We will continue to develop transient absorption microscopy and time-resolved optical emission microscopy with simultaneous high temporal and spatial resolution, each of which complements our efforts with UEM. These optical microscopies will be used to address several areas in the transient response of materials, including effects that are triggered inhomogeneously, such as energy migration between domains in polycrystalline solids and transient excitations of materials that involve thermal dissipation. Multiple classes of materials problems and sample types prompt staff and user interest in UOM. Chief among these are small lateral extent or spatially varying samples with inhomogeneities or variations in electronic properties (*Nature Comm.* **11**, 4442 [2020]). Often such inhomogeneities play key roles in the local nucleation and triggering of events, such as charge separation, energy funneling, or phase transitions, including metal-to-insulator transitions. UOM offers the spatial and temporal resolution needed for such studies. Characterizing the time scale and channels into which energy flows upon impulsive excitation is fundamental to a wide range of non-equilibrium 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 the femtosecond to picosecond time scales. Our interest here lies in gaining a fundamental understanding and control of dynamic electron–phonon processes, with the broader goals of tailoring energy flow within nanostructured materials and controlling spectral evolution of carriers and phonons. Concomitantly, we will perform theoretical modeling of non-equilibrium 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.

Moving to the UEM, this tool was commissioned as a user instrument in March 2021 (Figure 2-4). It combines a state-of-the-art, high-repetition-rate, tunable femtosecond laser with selectable pump wavelength from 325 to 2,000 nm and a synchronous laser-pumped, pulsed TEM that is outfitted with high-sensitivity cameras and electron energy filtering. In the stroboscopic UEM mode, the instrument delivers up to 470-fs temporal resolution, 0.5-eV energy resolution, and 1–1,000 electrons per pulse (depending on time-resolution needs). This tool creates a unique microscopic perspective on the local origins of transient and non-equilibrium material response, complementing ultrafast spectroscopic and momentum-resolved techniques both for CNM staff and the broader user community. The UEM provides the means to evaluate sample

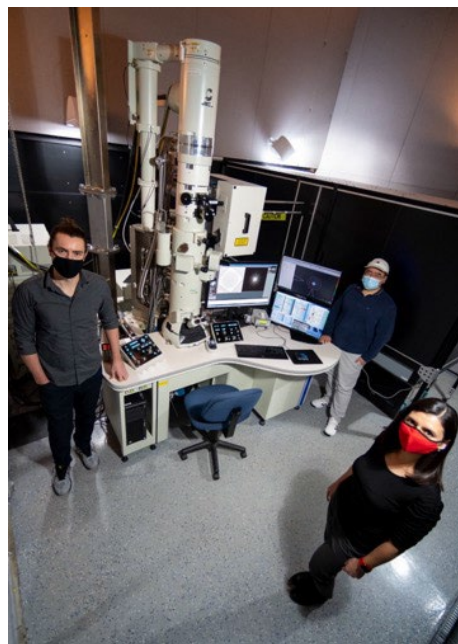


Figure 2-4: The Ultrafast Electron Microscope, shown with Tom Gage (left), Haihua Liu (middle), and Ilke Arslan (right). The ultrafast lasers that produce the pulses of electrons are in the black laser hut on the right.

changes spatially (with sub-nanometer resolution) and temporally with regard to real-space local structure, reciprocal space (via electron diffraction), charge distribution, and local electric field on ultrafast time scales. 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. Due to its complexity, this type of system to date has been available only to a few research groups that have specialized in technique development. However, we have the opportunity to harness the potential of this investment on behalf of a broad user community and staff, advancing in parallel many areas of nanoscience through the improved understanding of transient processes, such as in exciton localization, short-lived metastable phases, photo-induced segregation, dynamics in topological materials, plasmonic systems, molecular motors, magnetic fluctuations, to name a few.

We will work in the coming years to develop novel sample environments and routes of sample excitation of fundamental and device relevance by developing ultrafast mechanical and electrical triggering mechanisms in addition to a variable-delay pump-pump-probe mode. Combined with ultrafast probing, this will permit insights into non-equilibrium 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.

Building upon the HXN advances described in the Quantum Coherence by Design theme, we are also planning to upgrade our HXN for time-resolved nanobeam Bragg ptychography to fully utilize the upgraded source parameters of APS-U and create a unique visualization tool for time-resolved microscopy at high spatial resolution. We will be synchronizing observed dynamic material behavior with 3D visualizations created by scanning X-ray diffraction microscopy using 100-ps synchrotron X-ray pulses. Our goal is to create a 4D ptychography approach capable of imaging strain volumes with nanoscale (~20-30 nm) real-space voxel resolution at 100-ps time resolution. We will be able to detect, for example, time-resolved strain induced by ultrafast electrical, acoustic, or optical stimulation of defects in materials. The first steps in this development using the pre-upgraded APS source have recently been demonstrated at the HXN in collaboration with scientists from Argonne's Materials Science Division (*PNAS* **119**, e2118597119 [2022]), establishing the potential of this approach for a nanoscale understanding of ultrafast transition pathways for optically driven phase transitions. This capability can more broadly contribute to the understanding and control of dynamic electron-phonon processes in energy materials, as well as dissipation and decoherence in quantum materials, and enable us to study the roles of defects or inhomogeneities in triggering materials phenomena within large volumes. Our further planned development of AI-enabled correlative methodologies that broadly combine our *in-situ* time-resolved electron and X-ray microscopy capabilities will uniquely enable progress in these areas through correlative imaging of chemical heterogeneity with structural phase and strain to understand local perturbations in energy conversion within complex materials for quantum transduction, energy storage, harvesting, and catalysis.

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. The expertise in the CNM 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*.

In the *Interfaces for Emergent Properties* thrust, we will design strategies for fabricating varied (hetero) interfaces that showcase enhanced functionalities across various domains. We will utilize advanced *in-situ* and *ex-situ* probing techniques at the atomic scale, as well as computational and theoretical approaches. Theory is necessary to model these systems accurately and predict the performance of heterointerfaces with precision. Our research has resulted in new basic science understanding of novel interfaces with exciting functionalities. An example is the use of STM to observe anisotropic friction between an organic molecule and an atomically flat metal surface. The result is novel because normally friction is linearly proportional to the contact area between the molecule and surface, but in the case of the molecule sexiphenyl (6P) on an Ag(111) surface, the lateral force for moving the molecule along the long axis is found to be about half the lateral force needed to move the molecule along the short axis (Figure 2-5). The origins of this observation are linked to the one-dimensional structure of 6P and supported by molecular dynamics simulations (*Nano Lett.* **21**, 6391 [2021]). A second example of work in this thrust is the observation of plasmonic coupling at a metal nanostructure-graphene interface using the UEM (*Nano Lett.* **21**, 5842 [2021]).

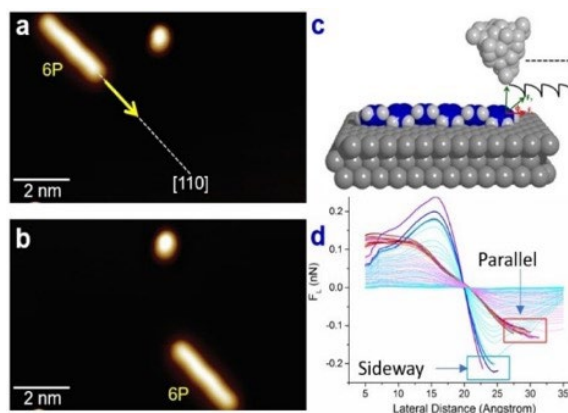


Figure 2-5: (a,b) Schematic of 6P molecule moved by the STM/AFM tip; (c) schematic of the STM experiment; (d) measured force curves.

Future work for this thrust will utilize many of our most advanced tools to reach new understanding of nanostructured interfaces. One example is to further understand energy dissipation at tribological interfaces to include high-entropy alloys and the Mxene family, in which we have demonstrated superlubricity (*Materials Today Advances* **9**, 100133 [2021]). Our approach will involve utilizing *in-situ* and *ex-situ* techniques across different length scales. For example, the *in-situ* TEM Picolindenter will enable nanoscale observation of tribological interfaces. Additionally, we will employ a multifunctional tribometer integrated with Raman spectroscopy and a confocal profilometer for macroscopic studies, offering a holistic understanding of mechanochemical processes at sliding interfaces. Atomistic simulations with the aim of extracting the precise mechanisms governing friction and wear will be performed. Other plans include using the 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.

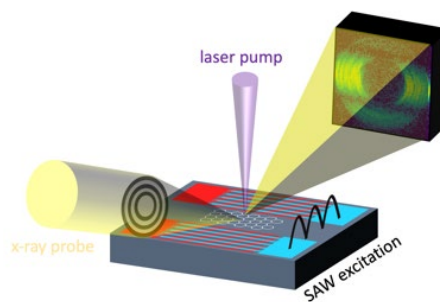


Figure 2-6: Schematic of the surface acoustic wave-laser pump X-ray probe experiment.

In the *Assembly for Emergent Properties* thrust, our objective is to unravel the intricate interactions among material assemblies at the interfaces down to the atomic scale. An example is that we have demonstrated with collaborators a new optogenetic method involving the nano-bio interface, which involves stimulation of neurons deep within the brain by means of injected nanoparticles that light up when exposed to X-rays (nanoscintillators) and would eliminate an invasive brain surgery currently in use (*ACS Nano* **15**, 5201 [2021]). We also have extensively studied the impact of ligands and solvents on nanoparticle assemblies (*J. Am. Chem. Soc.* **141**, 16651 [2019]).

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 which are of great potential relevance to microelectronics. We will leverage the unique characterization facilities at CNM and APS to probe the structural and electronic properties of the 3D/2D materials interfaces to understand the fundamental mechanism of charge transport. We will also use *in-situ* transmission electron microscopy (TEM) to correlate the transport properties of devices made from multilayer structures. In efforts connecting with the AI/ML-Accelerated Analytics and Automation theme, we will pursue an optimized algorithm for data reconstruction to better understand the interface structure in 3D/2D heterostructures.

In the *Fabrication for Emergent Properties* thrust, we manipulate materials or systems to exploit emergent phenomena for specific purposes such as mechanical, plasmonic, or quantum applications. The focus is to advance our knowledge of the understanding of material interfaces that enable guided improvement to the functionalities of the system or realization of entirely new phenomena. We have shown new approaches to fabricate high-performance resistive memory devices by synthesizing ultraporous oxide dielectrics (*ACS Nano* **15**, 4155 [2021]) and understanding fundamental limits to fabricate strain-free, ultrathin nanomechanical resonators based on silicon (*Nano Lett.* **20**, 5693[2020]). This work is in collaboration with the AI/ML-Accelerated Analytics and Automation theme, where we have developed, for example, DFT models for mixed dimensional heterostructures of interest for many types of devices, including field-effect transistors, sensors, and light-emitting diodes. We have even made advances in reconfigurable perovskite/nickelate electronics for AI applications (*Science* **375**, 533 [2022]).

Our future endeavors in this thrust will involve new fabrication strategies to create novel superconducting quantum circuits for improving the single electron on solid neon qubits by deterministically controlling single-electron trapping. In another example, we will fabricate meta-interfaces between metals and dielectrics to realize the extreme local field enhancement or guidance of an electromagnetic field at sub-wavelength nanostructures. We will also utilize the UEM to explore the spatiotemporal properties of surface plasmon polaritons (SPPs) that propagate in these structures. The UEM allows for exploring dimensions far smaller than traditional diffraction-limited optical microscopy allows. SPPs are of interest for a variety of technologies, including nanoscale photonic circuits, biosensing, and optical communication.

Theme V—Nanoscale Discovery for a Sustainable Energy Future

In this theme, we seek to leverage our leadership in computational modeling, advanced nanomaterial synthesis, and state-of-the-art experimental characterization to advance basic science and technologies relevant to clean energy. This thematic research has three thrusts: *Energy Storage*, *Energy Capture and Conversion*, and *Nanoscience for a Circular Carbon Economy*.

In the *Energy Storage* thrust, we are advancing fundamental understanding of batteries and energy storage platforms to directly impact clean energy technology. We use our state-of-the-art capabilities that include advanced TEM and the CNM/APS-based HXN to structurally characterize battery materials and interfaces and to link the findings to improved performance. With CNM users, we are advancing energy storage systems in areas that include improved electrolytes for lithium-air batteries (*Science* **379**, 499-504 [2023]). Collaborating with APS and our users, we used advanced synchrotron and 3D electron diffraction to detail decay mechanisms for promising Li-rich oxide cathodes (*Nature* **606**, 305 [2022]). We are also using new electron microscopy approaches that enable the study of the morphological evolution of anode materials in solid-state batteries at the single nanoparticle level during operation (*Nanotechnology* **34** 235705 [2023]).

For future work, we will continue to apply advanced characterization techniques to better understand the physics and chemistry of battery materials. One planned focus area is to use correlative electron and X-ray imaging to battery materials. Here, electron microscopy will provide structural imaging of the sample at the atomic level while synchrotron-based X-ray microscopy will provide sensitive strain information.

Together, the two offer a comprehensive view into the structural degradation and mechanical failure mechanisms of anodes, cathodes, and solid-state electrolyte materials.

In the *Energy Capture and Conversion* thrust, our goal is to collaboratively pioneer advancements in solar, photocatalysis, electrocatalysis, and energy conversion to provide the fundamental understanding needed to advance and optimize our ability to harvest and convert clean energy. For example, with our users we are applying advanced TEM characterization to reveal the structure-function reasons why an earth-abundant cobalt oxide material, doped with La and Mn ions, can function as an electrocatalyst for hydrolysis of water (*Science* **380**, 609 [2023]). We are also developing novel nanoparticle-purple membrane hybrid systems for light harvesting (*Adv. Funct. Mater.* **29**, 1904899 [2019]).

We plan to advance catalyst science through correlative studies of gas flow with electron- and X-ray microscopy as well as ambient pressure X-ray photoelectron spectroscopy (XPS), a recently procured capability scheduled for arrival in FY 2025. With this combination we will focus on catalysts for CO₂ reduction and hydrogen generation by taking advantage of both imaging and spectroscopy from high energy electrons and X-rays (Figure 2-7). We will also synthesize and characterize catalytic materials for the hydrogen oxidation reaction using the Polybot described in the AI/ML-Accelerated Analytics and Automation section.

Finally, in the *Nanoscience for a Circular Carbon Economy* thrust, CNM combines advanced computational modeling with novel material synthesis and state-of-the-art characterization to understand and exploit the relationship between nanoscale structure and local environments aimed towards carbon capture, conversion, and upcycling. As an example of our accomplishments in this area, we recently studied the catalyst Cu₂O, which is known to reduce CO₂ to methanol. A novel nanoreactor was developed that enabled studies of the same single Cu₂O nanoparticle under operating conditions, which used both advanced electron microscopy and X-ray fluorescence microscopy at the CNM/APS HXN (*Nature Energy* **4**, 957 [2019]) – Web of Science highly cited article). This study definitively showed that the (110) facet is the active surface for CO₂ reduction, while the (100) facet is inactive. This is an example of leveraging multiple facilities to enable a unique basic science study of a technologically important process. In a second experiment, we synthesized hollow TiO₂ nanocages functionalized with Pd, and then coated this with a purple membrane containing bacteriorhodopsin. Under illumination, we showed that bacteriorhodopsin functioned to pump protons across the hybrid membrane and reduce CO₂ (*J. Am. Chem. Soc.* **141**, 11811 [2019]). Electron paramagnetic resonance and transient absorption spectroscopies were used to establish the mechanism for CO₂ reduction.

With this background of accomplishment, research plans for the *Nanoscience for a Circular Carbon Economy* thrust will continue to include the engineering of biological pathways with man-made materials, and expand our targets to include nitrogen fixation, hydrogen production, and CO₂ reduction. We will also design eco-friendly peptide nanostructures to function as supramolecular bioelectronic materials. In addition, we will advance our characterization capabilities relevant to this area of research, such as by installing in FY 2025 an ambient pressure X-ray photoelectron spectrometer for structure-function characterization of surfaces relevant to catalysis. The ability to characterize materials while operating (*in operando*) will continue to be developed for this thematic area of research.

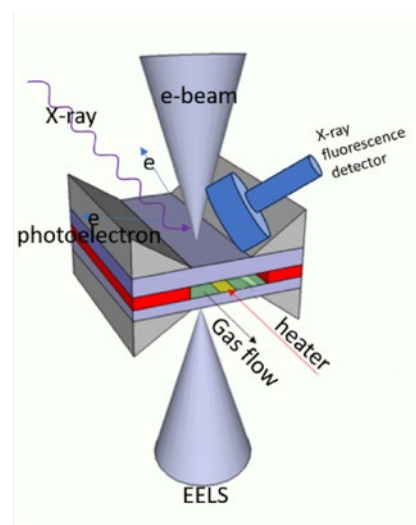


Figure 2-7: Nanoreactor for gas-solid reaction studies. It is compatible with TEM, X-ray microscopy, and XPS and also offers electron energy loss spectroscopy.

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-ft² cleanroom; the Carbon supercomputing cluster, which is being upgraded specifically for data-intensive ML workloads; quantum science capabilities designed to study single-photon as well as charge- and spin-based coherent systems; and the HXN jointly operated by CNM/APS. For a description of our many major capabilities, please see **Appendix 1.a**. For a complete list and description of all CNM capabilities, please visit our website [here](#).

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 display little to no usage. Our primary mechanism to upgrade our toolset is the recapitalization of a portion of our yearly funds. We are also currently acquiring equipment through the NSRC QIS grants and through the NSRC Major Items of Equipment (MIE) project. More detail on these mechanisms for acquiring tools is below.

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.

Another process through which new capabilities have been acquired is NSRC QIS grants. The CNM has received three of these grants. The first, entitled “Photon qubit entanglement and transduction,” provided major new capabilities in quantum optics, particularly enabling time-correlated single-photon counting microscopes in both the visible and near-infrared regimes. The near-infrared microscope includes single-photon detectors of ultrahigh-efficiency superconducting nanowires. Additionally, a magneto-optical microscope was constructed 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 given previously in the *Quantum Coherence by Design* theme section. Each of these tools is expected to be completed in FY 2024.

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 project, funded at \$80M, enables investment in major capabilities that are too large to be accommodated through NSRC recapitalization funds. The CNM will acquire four new tools via this project. The dynamic double-aberration corrected scanning transmission electron microscope (Dynamic DAC-STEM) as well as the transient photoelectron and cathodoluminescence spectroscopy (TPCS) tool will significantly add to our nanoscale dynamics research capabilities. The Dynamic DAC-STEM will be complementary to the UEM, by virtue of having higher spatial resolution, but will have longer time-scale dynamics capabilities (tens of microseconds and beyond). The TPCS tool will be placed at APS sector 29, with a vacuum highway between the TPCS instrument 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 be able to study dynamics with different contrast mechanisms. Since this tool can directly extract carrier energy dynamics, it is expected to complement our time-resolved optical capabilities in cases where 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 plasma-focused ion beam will also be acquired and will enable nanostructuring without concern for gallium-ion doping issues, which can limit electronic performance of a nanostructured device. It will also enable much faster materials preparation for TEM studies. Finally, the STM will give our users access to millikelvin temperatures, complementing our other variable temperature STMs and enabling detailed quantum state and spin state STM studies that were not possible before.

For additional detail and timelines, the tools that we plan to acquire through the three processes of recapitalization, NSRC QIS projects, and the NSRC MIE project are given in **Appendix 1.b**.

4. Operations

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

Staffing

The CNM opened for operations and began welcoming users in the fall of 2006. Since this time, the CNM has grown as a facility, with approximately 40 regular staff (research and technical support) members and 850 users annually. A detailed and updated organization chart can be found at the CNM website [here](#). The line management of the 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 the CNM spans and engages all groups. The groups and their respective group leaders are described below.

The Nanofabrication and Devices Group (NFD), with Group Leader Anirudha Sumant, specializes in the development and study of micro- and nanoscale systems with the goal of achieving 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.

The Nanoscale Synthesis and Characterization Group (NSC), with Group Leader Nathan Guisinger, 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.

The Nanophotonics and Biofunctional Structures Group (nPBS), with Group Leader Richard Schaller, seeks to understand and control light–matter interactions in nanomaterials. It does so 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. Through basic science advances in light–matter interactions, the group seeks to impact our thematic research and technologically important areas of nanoscience.

The Electron and X-ray Microscopy Group (EXM), with Group Leader Martin Holt, 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 the use of advanced electron and X-ray imaging, diffraction, and spectroscopic techniques coupled with data science-based approaches. Their research bridges the unique capabilities offered by the newly developed UEM and an HXN that will be enabled by the APS-Upgrade. The group also drives traditional strengths in high-resolution and *in-situ* quantitative electron microscopy.

The Theory and Modeling Group (TMG), with Group Leader Subramanian Sankaranarayanan, works on large-scale molecular dynamics, high-level electronic structure theory, AI/ML quantum and electrostatics theory, and multi-scale modeling and data science–based approaches to understand and predict a wide range of phenomena, including nanoscale tribology, thermal and charge transport, and quantum-entangled systems. It also plays a strong role in our efforts in autonomous synthesis as described in the AI/ML-Accelerated Analytics and Automation theme.

A facility of this size also requires dedicated personnel to support science and operations. These personnel, numbering approximately one dozen, provide for user program administration, IT (addressing computer administration, data management, and the development of operations software), safety, 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: (i) our ability, along with our users, to continue to perform world-class science; (ii) investments in differentiating and leading-edge research tools that attract the best scientific users; (iii) recruitment and retention of talented scientific staff; and (iv) importantly, our ability to anticipate and influence strategic areas that will define future nanomaterials research. These four objectives need to be accompanied by a realistic staffing plan and an investment plan that is compatible with projected budgets and turnover. Going forward, we plan to add research staff hires in key strategic areas that link to our thematic research in each of the following areas: clean energy and sustainability, AI/ML, advanced characterization, and QIS. Additionally, as our number of users continues to grow, we also intend to make new technical staff hires in the capabilities areas with the heaviest use that map to our strategic growth areas. The approximate rate of these hires during the next five years is 2 FTE for research staff and 2 FTE for technical staff for FY 2024 and FY 2025, followed by 1 FTE for research staff and 1 FTE for technical staff in FY 2026-FY 2028. Finally, we note that the CNM believes in a supportive and diverse work culture, and believes that it maximizes our research and user science output and impact. More details on our Diversity, Equity, Inclusion, and Accessibility (DEIA) efforts are given in **Appendix 2**.

Safety

CNM has responsibility for environment, safety, health, and quality assurance (ESHQ) aspects of the facility's 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 help CNM better ensure research productivity in conjunction with efficient implementation of the applicable ESHQ standards and requirements. The 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

The 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). This is 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, etc. The CNM implements the components of the CSPP to meet the requirements. In addition, CNM augments the 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:

1. Reliably capture and describe scientific data in a way that facilitates preservation and reuse.
2. Create quality metadata for data discovery, preservation, and provenance.
3. Design and implement interfaces for users to obtain and interact with data.
4. 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. The CNM also has a data-retention policy for user-generated data, which is described on the CNM website ([link](#)).

5. User Community

The CNM strives to attract a diverse 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 diversity of CNM users as a function of their affiliation, showing that slightly more than half of the approximately 850 users per year are from U.S. academia, with representation of non-Argonne users from international, industrial, and other government organizations as well. Figure 5-2 displays the diverse fields of research represented by CNM users.

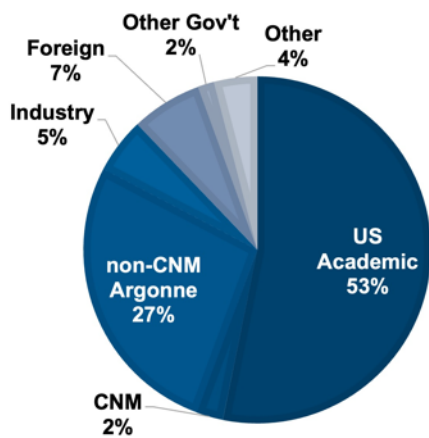


Figure 5-1: Institutional affiliations of CNM users by affiliation during FY 2023.

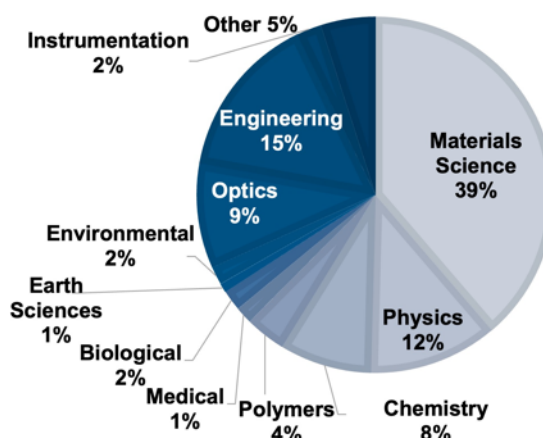


Figure 5-2: Fields of research identified by CNM users during FY 2023.

Our users, together with CNM’s research/scientific support staff, continue to have an excellent scientific impact, with peer-reviewed publications annually near or above 300 per year and with 55% published in journals having an impact factor greater than 7 (FY 2023). The global COVID-19 pandemic that began during FY 2020 impacted our ability to host our usual complement of users. However, demand was still strong, and we were able to accommodate the work of 631 unique users that year. Furthermore, in FY 2020 and FY 2021, we invested significantly in remote-access capabilities, which enabled users to remotely access more than 30 tools during this period. This effort resulted in the CNM’s ability to begin hosting more users in FY 2022 than during the pre-pandemic period. In FY 2023 the number of unique users grew to 850, with 509 onsite users and 341 remote users. We are continuing 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 the CNM.

User time is allocated through a proposal submission and review process in which the 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 will maximize our impact to science and benefit our users requires us to anticipate future user needs, as well as help shape future areas of focus in the nanosciences. Our future capability and facility upgrades are based upon prioritization of our 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 taking into account any new initiatives driven by national needs.

Discussions with our Scientific Advisory Committee, our 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 (for instance, the Office of Science Basic Research Needs Workshops and Roundtables), which provide an indication of future user needs. We also seek feedback from an annual user survey given 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, an Industrial Collaboration Committee formed and organized a successful workshop, CNM–Industry Collaboration Opportunities, at the CNM/APS annual user meeting to reach out to industry users. The purpose was to let them know about the capabilities and expertise available at CNM and accelerate new collaborations with industry users. This type of outreach to industry will continue. Industrial partners that have worked with us include major organizations such as John Crane, Inc., Magna International, and Boeing. Smaller partner companies include Euclid Tech Labs, Sentient Science, Axion Technologies, QDIR, Lam Research, Rigaku, Creative Microtech, Frore Systems (a Silicon Valley startup), Alcorix and Iris Light Tech (a spin-off from CNM).

We note that 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 will 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 to cutting-edge new technologies. Finally, research and development on “digital twins” will allow users to explore characterization experiments and conditions before arrival at the CNM, enabling users to jump start their visit and efficiently target the experiments most likely to succeed.

Finally, we emphasize that CNM seeks to provide a welcoming environment for diverse users and staff across different career stages, institutions, and nationalities (**Appendix 2**). We recently established a DEIA committee that will further enhance feedback between users and CNM staff, to continue to ensure a positive and respectful workplace culture. We are also planning additional outreach to minority serving institutions, as well as planning to establish formal opportunities for students at such institutions to work at the CNM.

Appendix 1.a: Major CNM Capabilities

The CNM maintains a large suite of capabilities, while regularly upgrading or procuring new capabilities. A full list of capabilities can be found at our website ([link](#)). Given here are detailed descriptions of major CNM capabilities that have been developed by our staff, where additional descriptions are warranted to aid users who may be interested in accessing them.

Quantum Information Science (QIS) Capabilities

For the past several years, the CNM has added several new tools focusing on QIS research, dramatically impacting our activities within the Quantum Coherence by Design theme. The 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 (DR)-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. It is the first millikelvin lab within the NSRCs. The system is equipped with microwave spectroscopy capabilities for spin-based studies, and soon, a femtosecond ultrafast laser system will be integrated with the DR system. A second tool, the adiabatic demagnetization refrigerator (ADR), became available to users in the October 2021 user proposal call. The ADR offers faster cool-down 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 is a comprehensive suite of user tools being developed for the study of quantum optics and hybrid quantum networks linking photons, spins, and magnons. The 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. Already commissioned and available for users is a photon correlation microscope that enables time-gated photon correlation (and a 9-T 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 nm to 1300 nm, as well as visible and near-infrared 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. In particular, 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.

Ultrafast Electron Microscopy (UEM) Laboratory

The UEM was installed in spring 2019 and began full user operations in 2021 as the first user tool for UEM within the NSRCs. This tool, in its final form, allows users to access time-resolved stroboscopic imaging, diffraction, and spectroscopy/spectral imaging capabilities, built using a combination of commercial vendors for transmission electron microscopes (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 2000 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 multi-modal multi-platform data synthesis.

Artificial Intelligence (AI) for Materials Science Capabilities

CNM has set forth a comprehensive software and hardware upgrade plan, which 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 the AI/ML-Accelerated Analytics and Automation theme section. A few more details are given below:

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

In this project, we are developing a computer vision-based software tool that will enable close to real-time interpretation of images generated from electron and scanning probe microscopies. FANTASTX will ingest experimental images as input and make 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. To start, this capability will be deployed in the EXM group.

BLAST (Bridging length-scales via atomistic simulation toolkit)

Molecular modeling is a powerful tool today. Historically, however, a gulf exists 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. Users currently do not have the flexibility to adapt these predefined potential models to problems of their interest. BLAST, a computational workflow tool, will overcome this barrier by allowing users to create their own models by providing 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 will be able to 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.

Our tasks also include development of a user-friendly, common-platform graphical user interface (GUI) for FANTASTX and BLAST, with GUI development being subcontracted. As of October 2021, we have a beta version of BLAST available to expert users and are currently in the process of licensing the software to Sentient Science. We also built a GUI and are currently carrying out GUI integration with the backend.

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 GPU (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 plan to continue upgrading the Carbon Computer Cluster as technology evolves.

Superlubricity Science Laboratory

For several years, CNM scientists have been exploring and demonstrating 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 the area of superlubricity science at the nanoscale.

A Superlubricity Science Laboratory has recently been configured to include a multifunctional tribometer with integrated confocal microscopy and Raman spectroscopy. We added new capabilities that will allow us to: (i) carry out *in-situ* TEM of tribological interfaces and changes upon loading and (ii) assess the wear/friction behavior of two-dimensional materials and nanomaterials at elevated temperatures (~500°C), uncovering the detailed wear/friction behaviors of these materials that are unknown today. Combining these new 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, through funding (~\$9 million) from Argonne, the CNM cleanroom was expanded from 12,000 ft² to ~18,000 ft². 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 the space. This expansion has 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 atomic force microscope for metrology, replacement of a critical point dryer for micro-electromechanical systems release, a thermal evaporation system from Angstrom, and others.

Appendix 1.b: Future Capability Enhancements at the CNM

As described in the strategic plan, the CNM acquires new tools primarily through three processes that include “recapitalization” with up to 10% of CNM’s operating funds each year, through external grants (particularly NSRC QIS infrastructure grants), and through the DOE Major Items of Equipment (MIE) project. The equipment we are planning to acquire is given in the table below, separated into time frames of near term (1-2 years) and long term (3-5 years). Many of these items address key priority areas such as AI/ML and autonomous synthesis, as well as replacement of aging capabilities with upgraded, state-of-the-art tools. Some examples of the tools planned include an automated profilometer station that can be integrated into the autonomous Polybot (described in Section 2) to provide extremely accurate, repeatable, and reproducible metrology for surface characterizations. This is important because surface morphology and thickness are key characteristics for discovery of nanoscale thin film materials, which can be used for microelectronics and energy storage applications. Also contributing to this research direction is the planned acquisition of a Plate Reader Research Hub for automated materials database development. This is a suite of automated tools for basic, but systematic sample preparation and characterization in plate reader format. This would fulfill the needs of nano-bio users interested in high-throughput sample preparation and characterization as well as fast database curation. Some of the tools are chosen for continuing to build on our areas of strength, such as dynamics studies, which include the transient photoelectron and cathodoluminescence system and the transient absorption microscope equipped with a high repetition-rate laser system for probing small materials with low energy pulses at a high rate of signal averaging. Characterization tools heavily requested by users, such as the X-ray photoelectron spectroscopy tool, are also planned for procurement. Additional details and motivations for many of these tools can be found within the strategic plan, particularly for the two NSRC QIS-funded tools (described in Section 2) and for the four MIE-funded tools (described in Section 3).

An additional exciting facilities upgrade, designed to support our diverse set of tools, reduce costs, and conserve helium (He), is that we are installing a He recovery system and a liquefaction plant capable of serving the CNM’s current and projected needs. Helium gas recovery drops are located in the relevant laboratories to recover boiloff from operating cryostats and bleedoff from storage dewars. The He gas is piped to the fan loft area above the cleanroom (Bldg. 440/C201), where a 300 cubic foot storage bag collects He gas for compression and storage in six medium pressure (400 psi) storage dewars. The He gas will then be purified and reliquefied at the rate of ~80 L/day and stored in a 500 L dewar. From there, transport dewars can be refilled and delivered back to the laboratories for the operation of cryogenic instruments. The installation covers a total of 460 square feet. The system will be installed in FY 2024.

Tool	Source of Funds	1-2 years	3-5 years	Function
XPRESS 3X MK2 8 Channel Readout Electronics	Recap	X		Enables high speed X-ray fluorescence imaging at the Hard X-ray Nanoprobe; upgrade is needed to benefit from photon flux increase of APS-U
Lesker Sputtering CMS18: RF Subsystem	Recap	X		Add-on to an existing sputtering tool that enables reliable sputtering of dielectric films – original capability for dielectric films has now failed
Femtosecond Pulse Compressor with Frequency Resolved Optical Gating	Recap	X		Compresses optical pulse durations on our femtosecond spectrometer from 35fs to 5 fs to extend range of dynamics that can be explored

Tool	Source of Funds	1-2 years	3-5 years	Function
Temperature Stage for Bruker D8 Discover X-ray Diffractometer	Recap	X		Adds temperature control capability to our newly acquired Bruker D8 diffractometer; adds additional experimental capabilities for users
Transient Absorption Microscope with High Repetition Rate Laser	Recap	X		Permits examination of transient dynamics and spectral response of small samples
Nanosecond Transient Absorption Laser Upgrade	Recap	X		A tunable pump source is added to the nanosecond spectrometer to enable many more samples to be studied
THz Spectrometer and Imager	Recap	X		Time-domain terahertz spectrometer capable of 0.5 to 22THz measurements with ~4 spectra/s and 100micron spatial resolution (2.7 GHz spectral resolution)
X-ray Fluorescence Analyzer (XRF)	Recap	X		XRF provides rapid, non-destructive, multi-element analyses of many materials
Quantum Design Dynacool 14 Tesla Physical Properties Measurement System (PPMS)	Recap	X		Replaces a heavily used, aging PPMS system. Additional utility is gained with a strong magnet (14T) and closed-cycle LHe cooling, saving considerable \$ and time relative to older system.
Heidelberg MLA 150 Advanced Maskless Aligner	Recap	X		Complements an existing, heavily used older version of this tool; new version has high spatial resolution that enables decommissioning the old Raith e-beam lithography tool
Ambient Pressure X-ray Photoelectron Spectrometer	Recap	X		Enables XPS of surfaces and liquids at ambient conditions as compared to a traditional UHV system; dynamics of surface process related to clean energy research is a priority
Gallium Focused Ion Beam (FIB) tool	Recap	X		Replacement of an aging FIB to be primarily used for TEM sample preparation
Helium Recovery and Liquefaction System	Recap	X		Needed for continuing operation of helium cryostat-based user tools, from both a supply and cost perspective
Atomic Quantum Information Surface Science (AQuISS) Lab	NSRC QIS	X		Scanning probe tool for controlling and characterizing optically active spin quantum systems near surfaces
Quantum Emitter Electron Nanomaterial Microscope (QuEEN-M)	NSRC QIS	X		A TEM that integrates time-resolved cathodoluminescence to characterize the electronic structure of quantum emitters

Tool	Source of Funds	1-2 years	3-5 years	Function
Dynamic Double-Aberration Corrected Scanning Transmission Electron Microscope (Dynamic DAC-STEM)	MIE	X		Provides high spatial resolution combined with longer-time dynamics capabilities complementary to UEM
Multibeam Ion Microscope	MIE	X		Complements Ga ⁺ FIB with state-of-the-art plasma FIB
Transient Photoelectron and Cathodoluminescence Spectrometer (TPCS)	MIE	X		Gives dynamics of carrier energies directly to complement optical measurements (placed at APS to enable structure-function correlation studies)
A Microscope Capable of Single Spin Imaging (mK-STM)	MIE	X		Gives access to milli-Kelvin scanning tunneling microscopy to complement our suite of variable temperature STMs
Magnetic Cryostat Transient Absorption System	Recap		X	Permits examinations of carrier spin dynamics
Plate Reader Research Hub for Automated Materials Database Development	Recap		X	Suite of automated tools for basic but systematic sample preparation and characterization in plate reader format
Automated Profilometer Station	Recap		X	To be integrated into Polybot to provide extremely accurate, repeatable, and reproducible metrology for surface characterizations

Appendix 2: Diversity, Equity, Inclusion and Accessibility at the CNM

At Argonne and the CNM, we recognize that our future success depends on our ability to recruit and retain a diverse workforce. Bringing together people whose cultural and intellectual backgrounds equip them to look at a problem from different viewpoints is key to collaboration and innovation. Creating a diverse, equitable, and inclusive environment is not a singular project or one-time initiative. It is an ongoing and constantly evolving effort that involves everyone in the CNM and includes all aspects of our user support, our research, and our development projects.

Argonne has an active and ongoing Diversity, Equity, Inclusion, and Accessibility (DEIA) program, the vision of which is to create a safe, welcoming, diverse, and inclusive environment for all Lab employees. This vision is complemented by Argonne's commitment to creating systemic equity to ensure all Lab employees are treated fairly. Each year, the Laboratory Director works closely with Laboratory leadership and Argonne's Leadership Institute to develop a strategy for DEIA at the Laboratory, which is manifested in a number of documents, including Argonne's Annual DOE DEIA Plan. The CNM's Promoting Inclusive and Equitable Research (PIER) plan is in line with Argonne's core values and complements the DEIA activities and initiatives of Argonne National Laboratory and the Physical Science and Engineering Directorate.

To help address DEIA challenges, the Nanoscience and Technology Division (NST) DEIA Council was established as an advisory body to the NST/CNM leadership in 2021. (Note that NST is the parent division of the CNM). The purpose of this Council is to create a safe and welcoming work environment for everyone, regardless of their race, color, national origin, religion, gender, gender identity, sexual orientation, age, or disability. In alignment with Argonne's goals in the Argonne DEIA Strategic Plan, the CNM PIER plan sets forth the following goals:

Goal 1: Ensuring employees have a sense that they are valued, supported, and included.

The day-to-day culture of NST/CNM should be one of allyship, fairness, and collaboration, where everyone is valued both personally and professionally, with the goal of creating a physically and psychologically safe work environment, as well as inclusion of diverse thoughts, opinions, knowledge, and expertise.

Goal 2: Increasing equity among employees and providing equitable opportunities for advancement.

NST/CNM staff at all levels should have equitable opportunities for advancement. To support this, each supervisor is dedicated to discussing staff goals several times per year and providing opportunities for development. When opportunities arise, supervisors will be active in nominating their staff.

Goal 3: Expanding professional development opportunities for employees to grow.

We will take a proactive role in fostering professional, career development and recognition of NST/CNM staff. We have instituted Deputy Group Leader positions to help train the next generation of potential group leaders. We will continue to nominate our staff for leadership opportunities across the Argonne campus, as well as external to the Laboratory. We will support training courses supported by the Argonne Leadership Institute, as well as external courses (including those that take place at conferences) that staff desire to take to advance their career development.

Goal 4: Creating a climate for diverse recruiting.

NST/CNM will continue exploring multiple avenues for talent acquisition and development to promote fairness and diversity in the recruitment, support, and retention of an efficient workforce, with the long-term goal of surpassing the national averages in demographic statistics in STEM-related fields. We are committed to equity in hiring, compensation, and professional development.

Goal 5 (CNM-specific for Users): Ensuring users feel valued, supported, included, and heard.

As we grow our user community, we strive to promote equitable access to the CNM. Many underrepresented users and underserved academic institutions, such as minority serving institutions (MSI), may not even be aware of the resources available to them at these user facilities. The CNM plans to target outreach to MSIs by giving talks at specific universities and joining MSI-specific professional groups. We plan to provide information about the CNM, tools and resources available, guidance on how to submit a successful proposal, and funding opportunities for students. Two such opportunities at Argonne are the Science Undergraduate Laboratory Internship and the National Consortium for Graduate Degrees for Minorities in Engineering and Science Consortium.

Some actions that the NST/CNM DEI Council will take in order to advance the five goals discussed above are the following:

- Creating a CNM DEI Webpage for sharing all relevant information with staff and users (e.g., people, events, cultural observances, and strategic plan), which also includes an anonymous online suggestion box
- Regularly contributing to a DEI section in the CNM newsletter
- Collaborating with the NST/CNM hiring committees of any posted positions
- Conducting staff surveys
- Collaborating with the CNM User Executive Committee and the Scientific Advisory Committees
- Collaborating with the laboratory-wide DEI councils and Employee Resource Groups
- Promoting Argonne community outreach and educational programs
- Providing staff with information on DEI training opportunities and activities throughout Argonne

A diverse, equitable, and inclusive culture is associated with higher productivity, innovative solutions, employee engagement, and talent retention. We aim to broaden the participation of individuals from diverse backgrounds, including individuals historically underrepresented in the research community; to contribute to the goal of creating and maintaining an equitable, inclusive, encouraging, and professional training and research environment for users and employees; to support a sense of belonging among personnel; and to provide intentional mentorship and the associated mentoring resources. In addition, we aim to have the product of our research serve to create a better, equitable world.