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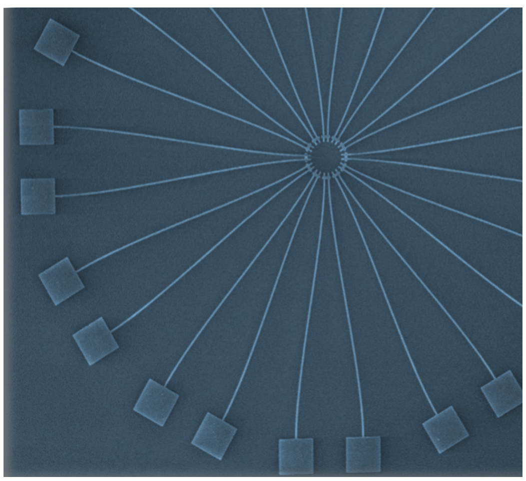
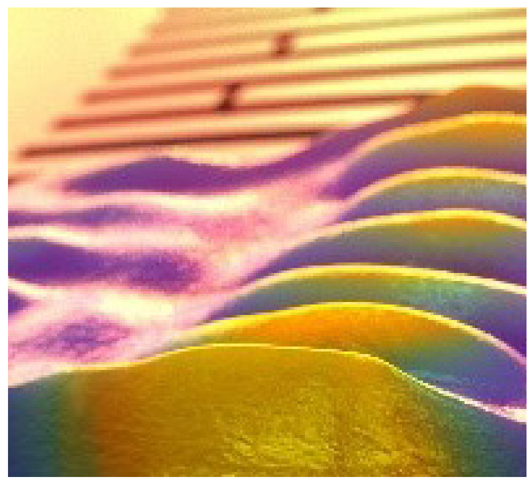
Argonne NATIONAL LABORATORY

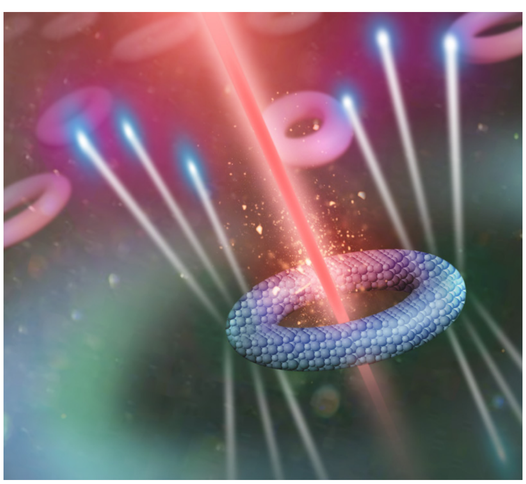
CENTER FOR NANOSCALE MATERIALS

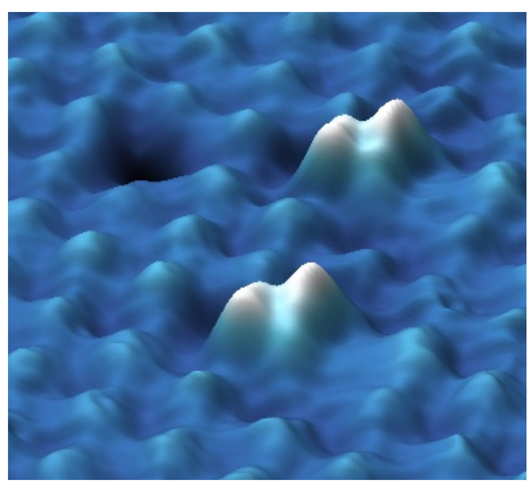
STRATEGIC PLAN

Fiscal Years 2021–2025









U.S. DEPARTMENT OF ENERGY

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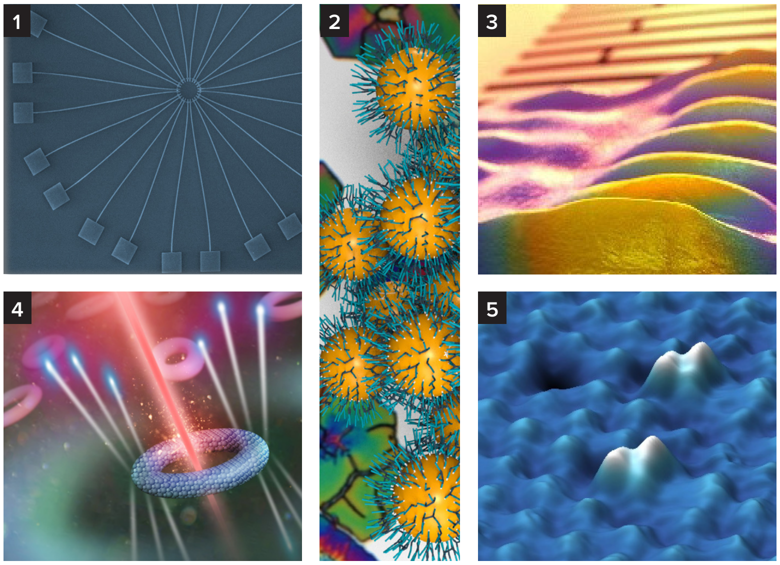
ON THE COVER



1. Circular array of superconducting single-electron transistors created by nanofabrication tools in the CNM cleanroom, including electron beam lithography, focused ion beam lithography, sputtering, and reactive ion etching. The width of one thin wire is 50 nm.
2. Coarse-grained molecular dynamics simulation showing superlattice of nanoparticles (yellow) stabilized by ligands (blue). Background image of nanoparticle superlattice crystals taken by optical microscopy. (*Nanoscale* **11**, 10655 [2019])
3. Three-dimensional rendering of time-varying lattice strain caused by focused surface acoustic waves used to manipulate spin defects in the quantum material silicon carbide (SiC). Image created in collaboration with University of Chicago at CNM/APS Hard X-ray Nanoprobe. (*Nature Commun*. **10** (1), 3386 [2019])
4. Depiction of a cadmium selenide (CdSe) 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])
5. Image from atomic-resolution ultrahigh vacuum scanning tunneling microscopy of the (111) surface of Cu_2O. Each small protrusion in this image is an unsaturated copper atom, while oxygen atoms (not seen) reside in between the Cu atoms. The black “hole” reveals a missing copper atom, and the triplets of elevated copper atoms indicate that the oxygen atom that should reside between them is missing.

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Executive Summary

Our vision for the Center for Nanoscale Materials (CNM) at Argonne National Laboratory (Argonne) is to continue to enhance its role as a world-leading research center and user facility in nanoscience, and to expand in areas that emphasize the discovery and integration of materials across different scales and at the extremes of temporal, spatial, and energy resolutions. This emphasis describes collectively the three scientific themes of our five-year Strategic Plan. The themes of the Strategic Plan connect the CNM research groups and inform our strategies for new scientific directions and for investments in staff, user engagement, equipment, and infrastructure.

CNM carries out research and develops its capabilities within three major strategic themes:

I. **Quantum Materials and Sensing**. The goal of this theme is to combine CNM's expertise in synthesis, fabrication, characterization, and theory on nanometer length scales to discover fundamental mechanisms and materials for quantum information and sensing. This theme includes the study of the fundamentals of sub-wavelength light localization, spins, and optically and electrically accessible defects in low-dimensional and bulk materials for quantum coherence and entanglement.

II. **Manipulating Nanoscale Interactions**. The goal of this theme is to study the mechanical forces and the electromagnetic interactions between nanoscale constituents at length scales that vary from the atomic to the sub-micron. These include manipulating and coupling nanomechanical elements or optical near fields, determining the origin of energy dissipation via friction at the nanoscale, simulating materials and defects from their inter-atomic interactions, and synthesizing hierarchical structures across different length scales.

III. **Nanoscale Dynamics**. The goal of this theme is to study excitation-driven energy flow and structural transitions in nanoscale materials on femtosecond to millisecond time scales over angstrom to macroscopic length scales. This includes, for example, the evolution of optical and electrical properties in materials in response to stimuli, study of reaction dynamics, and probing of exchange processes between excitations on the nanoscale. This theme leverages the rapid ongoing improvements in instrumentation for in-operando observation that enable multi-dimensional parameter measurements, including high-resolution spatiotemporal imaging using excitations such as electrons or photons.

Beginning in FY 2016, CNM initiated activities in three major areas where it believes future user and research interest will increase. The first is in materials for quantum information where, beginning in 2016, we hired five new staff scientists, in addition to significant investment in equipment. These investments correctly anticipated the extensive interest in quantum information science (QIS) that the research community has experienced since 2017. The second area is in ultrafast electron microscopy (nanoscale dynamics theme), where we have already started growing a new user base by being the first Nanoscale Research Center (NSRC) to offer user capabilities (currently available for experienced β-users but will be available as a general user tool in March 2021) for ultrafast electron microscopy (UEM). This tool, which we carefully designed and is now online, 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. The third area is in the use of artificial intelligence for science, where CNM scientists are developing tools and methods for faster and more accurate molecular modeling of materials and on-the-fly interpretation of electron and X-ray microscopy data. Of particular note is the CNM Theory and Modeling group's close relationship with the Argonne Leadership Computing Facility (ALCF). Working with the ALCF, we currently have access to Cerebras (commissioned in 2019), which is one of a new generation of hardware processors specifically configured for deep learning. We will also have access to Aurora (to be commissioned in 2021), the world's first exascale computer.

Research at CNM is closely tied to significant capabilities at the Advanced Photon Source (APS) and the ALCF. Research collaborations among APS, ALCF, and CNM are important differentiators of CNM and key factors in the development and implementation of our Strategic Plan. These distinguish CNM from the other four NSRCs operated by the Office of Basic Energy Sciences (BES) and other nanoscale science research efforts in the United States and abroad. Furthermore, researchers at CNM work closely with their counterparts in a number of Argonne divisions; chief among them are the Chemical Sciences and Engineering Division and the Materials Science Division in the Physical Sciences and Engineering Directorate and the Data Science and Learning Division in the Computing, Environment, and Life Sciences Directorate.

The research at CNM is only as good as its capabilities, staff, and users (Figure 1-1). Leveraging our relationships with some of the best research groups in the world, aggressively going after promising candidates, and recruiting selectively, we have been able to, and will continue to, attract world-class talent to CNM. These individuals with world-class promise bring fresh thinking to our scientific themes and user programs. Our outreach to users encompasses three principles. First, we listen to them carefully, and their feedback informs our capability acquisitions. Second, we strategically anticipate emerging directions in the nanosciences, and then position ourselves to intercept these directions as appropriate. As will be described later, our decision to expand quantum information sciences, artificial intelligence for science, and UEM research are examples of this strategy. Third, in the next five years, we seek to capitalize on new technologies and systems to reinvent CNM's approach to user facility activities. The intent is to streamline the user experience via automation, use business intelligence to target new users, and explore extended reality technologies in the use of experimental equipment and analysis. Our dedicated instrument scientists and staff, such as those involved with cleanroom nanofabrication and microscopy, continue to receive stellar feedback from our users.

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.

In this strategic plan, we provide a concise outline of our scientific vision, opportunities, activities, and organizational structure. This document will guide our path over the next five years, with the aim of preserving CNM as a world-class user facility, where we are ready to provide capabilities for user needs in the next two to five years, and where our scientists can help shape the future of research in the nanosciences.

1. Introduction

CNM provides expertise and capabilities that enhance research in synthesis, fabrication, characterization, and theory/simulation of materials at the nanoscale. It focuses on discovery, integration, and manipulation of nanoscale materials at the extremes of temporal, spatial, and energy resolution. CNM staff and facility users conduct research consistent with our three major themes: (i) Quantum Materials and Sensing, (ii) Manipulating Nanoscale Interactions, and (iii) Nanoscale Dynamics. CNM is equipped with unique and comprehensive capabilities in cleanroom-based nanofabrication; electron, X-ray, and scanning tunneling microscopies; optical and transport physics; and computational materials science.

CNM staff and users are strong contributors to the field of nanoscience and technology: during fiscal year (FY) 2019 the CNM hosted 599 unique users, and our users together with CNM's research/scientific support staff are well on track to publish more than 325 papers in peer-reviewed journals. See Figure 1-2 for a snapshot of user facility statistics at-a-glance. The facility has an annual budget of approximately $28 million and spends at least 10% of its budget annually on new scientific equipment.

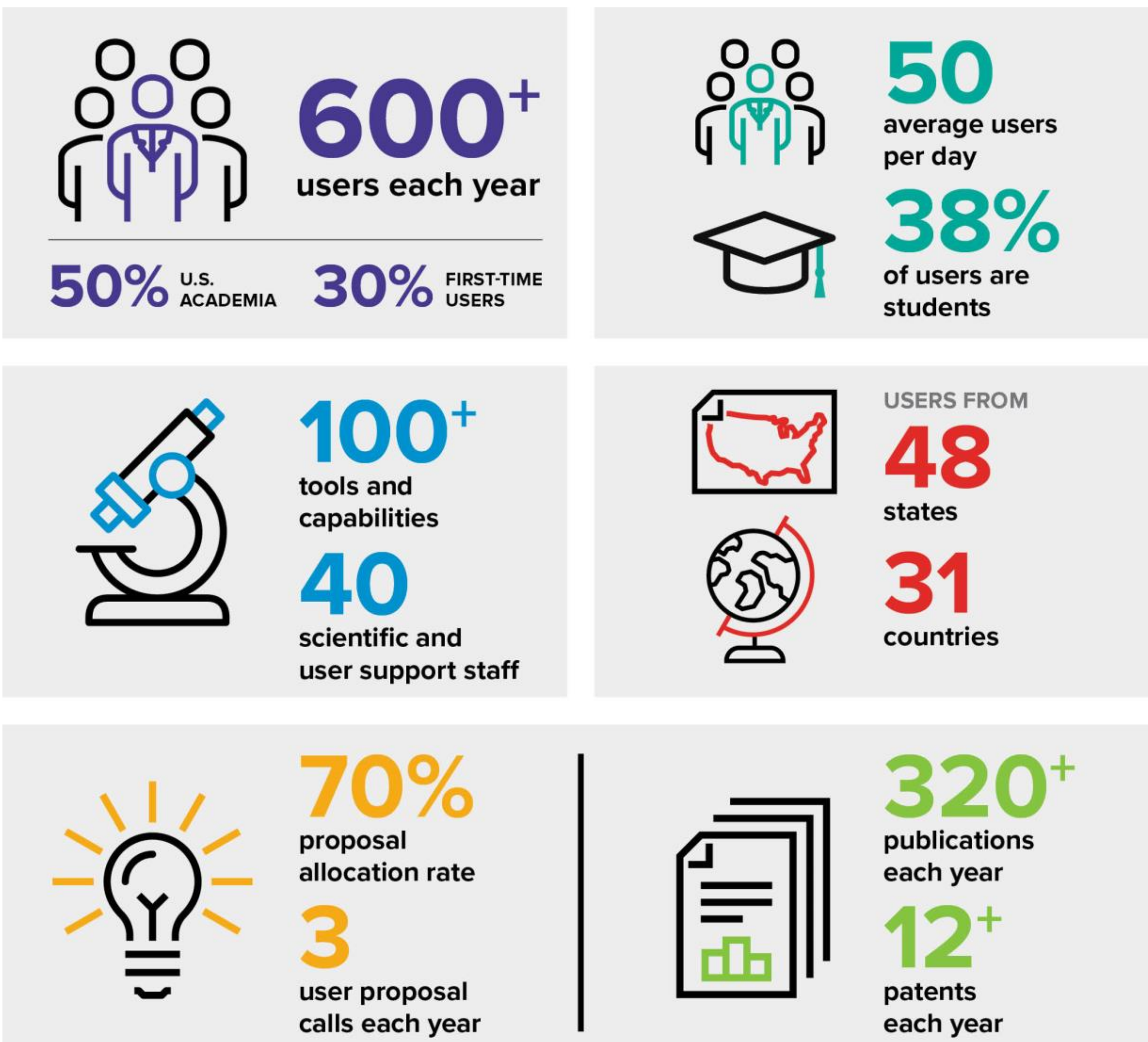

Figure 1-2: CNM at a glance. Numbers are recent averages except the number of states and countries, which are cumulative since 2007.

Figure 1-3 shows CNM staff. Over the past few years, CNM has made major strategic commitments to developing its research activities in materials for quantum information science, in UEM, and in the use of artificial intelligence for materials science. CNM's new UEM system, recently installed in 2019, will provide time-resolved stroboscopic imaging, diffraction, and spectroscopy/spectral imaging. It will be the first user facility of this kind in the United States and, to the best of our knowledge, in the world.

Figure 1-3: Center for Nanoscale Materials staff members in 2019.

In addition, CNM provides an array of capabilities, expertise, and tools to its users. These include optical spectroscopy from ultraviolet to terahertz at the extremes of spatial and time resolution; a full suite of variable-temperature scanning tunneling microscope capabilities; comprehensive nanofabrication capabilities in a newly expanded 18,000-ft^2 cleanroom; the Carbon supercomputing cluster, which will be upgraded specifically for data-intensive machine learning (ML) workloads; and a quantum systems laboratory that is currently being set up to study single-photon and spin-based coherent systems.

CNM works closely with the APS. We share two important capabilities that offer us uniqueness. The first is the Hard X-ray Nanoprobe (HXN), which enables high chemical and structural resolution (~20 nm) in three dimensions. The CNM/APS HXN is developing frontier capabilities for time-resolved operando structural microscopy, leveraging a combination of the sensitivity of nano-focused Bragg diffraction with the unique per-bunch-brightness of the APS storage ring.- This approach will benefit vastly from the 100-times improvement in beam brightness following the APS upgrade. The second capability is the synchrotron X-ray scanning tunneling microscope (SX-STM), which combines the strengths of high-brightness X-ray excitation and the spatial resolution of an STM with the goal of imaging chemical and magnetic contrast at the single-atom/molecule level. A dedicated beamline, designated XTIP, was recently completed at the APS to house the SX-STM. The SX-STM capability became available to users in August 2019. The use of this capability has grown rapidly, with the XTIP beamline supporting 14 user groups and 52 individual users as of September 2020.

Working within our three science themes, CNM scientists and our users are rapidly making numerous important scientific contributions. The examples below demonstrate the breadth of expertise and recent advances at the CNM. A representative example within the Quantum Materials and Sensing theme is the development of a stroboscopic imaging X-ray diffraction technique that demonstrated—for the first time—how sound, in the form of surface acoustic waves, can modulate solid-state qubits for quantum mechanical registers and transducers (*Nat. Phys.* **15**, 490 [2019]). A second example within this theme is research that shows how gold nanostructures can create highly localized strain fields in semiconductor monolayers to produce bright, single-photon emitters for quantum optics applications (*Nano Lett.* **20**, 5866 [2020]). A collaboration between CNM staff and users (Manipulating Nanoscale Interactions and Nanoscale Dynamics themes) detailed how graphene can reduce friction at moving interfaces, providing potential new pathways to improved energy efficiency and functionality for applications such as magnetic storage systems, micro- and nano-electromechanical systems, and mechanical devices in general (*Nano Lett.* **20**, 905 [2020]). A final example comes from the Nanoscale Dynamics theme, in which CNM users and staff worked together to understand the ultrafast dynamics of energetic electrons and holes created through optical excitation of gold nanoparticle/GaN composite systems, with potential applications to photocatalysis and photodetection (*Nat. Mat.* https://doi.org/10.1038/s41563-020-0737-1 [2020]). What are the areas of growth for our future? We highlight three opportunities that we believe will have the greatest scientific impact and user interest:

- The first is in the materials discovery, characterization, and engineering necessary to advance the quantum information sciences (part of the Quantum Materials and Sensing theme). Our decision to invest in new staff and equipment in this area since 2016 correctly anticipated the extensive interest in QIS that the research community has experienced recently. This is an area that matches very well with CNM's core expertise and leverages our traditional strengths in nanophotonics, nanofabrication, and operando characterization.
- The second area, one which greatly strengthens our Nanoscale Dynamics theme, focuses on the UEM system, which was installed in late FY 2019. We have already started growing a new user base by being the first NSRC to offer user capabilities for UEM. There is increasing interest in understanding materials phenomena such as ultra-fast (sub-picosecond) structural and chemical changes at the nanoscale in materials, and we believe that we will be able to capture an exciting area of emerging science here. Until now, this tool has been available only to a few research groups that specialize in technique development. Our decision to enter this area was also based on the core strengths that we have in the APS in ultra-fast phenomena, our expertise in ultrafast optics within CNM, and the complementarity that this technique will provide to our planned HXN research that, going forward, is geared towards transient X-ray microscopy.
- The third area is in the use of artificial intelligence for science, and this feeds into all three of our themes. Here, CNM scientists are developing tools and methods for faster and more accurate molecular modeling of materials, on-the-fly interpretation of electron and X-ray microscopy data, and the development of new approaches that will combine machine learning approaches with a physics basis.

CNM is also engaging actively in expanding the scope of its science toward industrial impact in the future, seeking opportunities beyond its industrial user program. During FY 2016–2020, CNM received five Department of Energy (DOE) Technology Commercialization Funding (TCF) grants in areas such as nanoscale superlubricity and artificial-intelligence-informed tools for molecular dynamics. Current industrial partners include major organizations such as John Crane, Inc.; Magna International; and Boeing. Partners also include smaller companies such as Euclid Tech Labs, Sentient Science, Axion Technologies, QDIR, Ragaku, Microtech, Frore Systems, a Silicon Valley startup, and Iris Light Tech, a spin-off from CNM.

2. CNM's Research Themes and Groups

CNM's scientific strategy is consolidated under the following three scientific themes that were defined in Section 1 and, for the sake of convenience, are reproduced below. Over the next five years, all of our research activity will be focused within these three themes.

I. ***Quantum Materials and Sensing.*** The goal of this theme is to combine CNM's expertise in synthesis, fabrication, characterization, and theory on nanometer length scales to discover fundamental mechanisms and materials for quantum information and sensing. This theme includes the study of the fundamentals of sub-wavelength light localization, spins, and optically and electrically accessible defects in low-dimensional and bulk materials for quantum coherence and entanglement.

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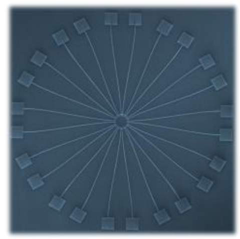
Within these themes, we specifically note three new topical areas for which we have ramped up effort and investment over the past two years. The first is in materials for quantum information science (part of Theme I). Starting from a position of almost no effort in this field in 2015, we hired five scientists who are QIS specialists over a 3-year period, and we have invested heavily in this area. The Department of Energy has also strongly supported this effort with the funding of the NSRC QIS grant entitled "Photon Qubit Entanglement and Transduction," which has provided approximately $5.1M in support for new QIS equipment and effort. The second is the use of artificial intelligence for materials discovery and characterization (part of Theme II), where we are now publishing significant work. The CNM received significant funding in this area, particularly with funding of an Early Career Research Proposal (ECRP) grant in 2020 for CNM staff member Maria Chan, entitled "Theory-informed Artificial Intelligence for Accelerating Materials Characterization," as well as involvement in four funded grants in 2020 (one as lead PI) for the DOE Funding Opportunity Announcement of "Data, Artificial Intelligence, and Machine Learning at DOE Scientific User Facilities." Both of these topics are of major growth interest to the DOE Office of Science, given the recent passage of the National Quantum Initiative Act in December 2018 and the Presidential Directive on Ensuring American Leadership in Artificial Intelligence in February 2019. CNM scientists are proactively involved in these new opportunities, sponsored by DOE, that involve the joint effort of universities, national labs, and industrial partners. The recent funding of the Q-NEXT (www.q-next.org) center, a DOE National Quantum Information Research Science Center led by Argonne is responsive to the NQI Act. The CNM now has considerable capabilities and expertise in characterization, fabrication, and theory relevant to QIS, which we believe will attract academic, national laboratory, and industrial participants in Q-NEXT, and perhaps from other quantum information science centers as well, to our user science program.

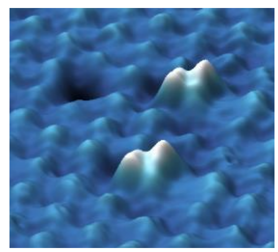
The third topic is the UEM (part of Theme III), where we anticipate a unique opportunity to establish a leadership footprint for CNM. Commercial column-based electron microscopes for UEM have just begun emerging over the past few years, and there are only a handful of such imaging microscopes worldwide, with only one such microscope in the U.S. (at the University of Minnesota) currently producing active publications. To the best of our knowledge, there are no such user facilities in the world today, while there is a growing need for this capability among users. The CNM UEM became operational in the summer of 2019. Together with our existing strengths in HXN microscopy, optical physics of nanostructures, near-field microscopies, and nanofabrication, CNM will continue to remain unique in its science offerings and capabilities. The UEM is currently working with β-users, and will become available to our general user base in early calendar year 2021.

CNM's scientific activities within the three scientific themes are carried out by five research groups, which interact closely with one another in carrying out their theme-based research. Each group is involved in research within all three themes. The group leaders are responsible for leading the scientific vision of their groups, for maintaining high standards for the staff, and for ensuring outstanding user research programs. Each group leader has line management responsibilities for the staff, laboratories, and safety. The groups and the respective group leaders are described below.

- **The Nanofabrication and Devices Group** (NFD), with Group Leader Anirudha Sumant, specializes in the fundamental science behind the development 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.

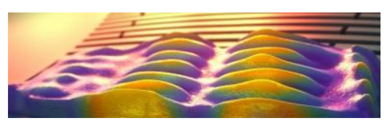


- **The Quantum and Energy Materials Group** (QEM), with Group Leader Nathan Guisinger, focuses on the synthesis and fundamental characterization of molecules and materials on nanometer to atomic length scales. This group employs molecular epitaxy, physical deposition, and chemical synthesis methods and uses 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 energy and quantum information science.

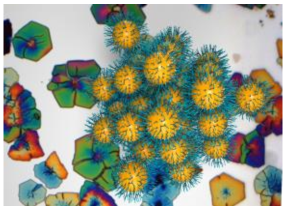


- **The Nanophotonics and Biofunctional Structures Group** (nPBS), with Interim Group Leader Richard Schaller, seeks to understand and control light–matter interactions in nanomaterials. It does so by studying the dynamics of photo-active processes through time-resolved spectroscopies and microscopies 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 technologically important areas that include quantum information science, energy conversion, and biosensing.

- **The Electron and X-ray Microscopy Group** (EXM), with Interim Group Leader Martin Holt, performs research to understand and control the structure and dynamic behavior of quantum- and energy-related materials at the atomic- to nano-scale via the use of advanced electron and X-ray imaging, diffraction, and spectroscopic techniques coupled with data science-based approaches. Their research leverages the unique capabilities offered by the newly developed UEM and the ultrafast HXN enabled by the APS-U.



- **The Theory and Modeling Group** (TMG), with Group Leader Subramanian Sankaranarayanan, works on large-scale molecular dynamics, high-level electronic structure theory, quantum and electrodynamics, 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.



3. Vision for Scientific Growth

With major investments made in equipment and infrastructure, and a number of newly hired staff scientists with world-class potential added to an established group of scientists responsible for our core strengths in nanophotonics, nanofabrication, microscopy, and synthesis, CNM is poised to continue to solidify its leadership position in worldwide nanoscience research. Our research will continue to be centered around three scientific themes—quantum materials and sensing, manipulating nanoscale interactions, and nanoscale dynamics. These themes have emerged from a carefully considered strategy, and they form the kernel of CNM's big bets for the future. We believe these areas will broadly address the future trajectory of nanoscience and will attract high-quality users. All of our plans, purchases, and hiring are premised upon the needs of our three scientific themes. Our thematic research and skills also mesh, as well as strengthen the larger Argonne strategic core strengths in computing, X-ray science, materials, and chemistry. 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 facilities 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.

The NSRCs are viewed as an important part of the national scientific infrastructure, as evidenced by numerous visits paid by representatives from U.S. academic and government institutions, as well as from industry and other national laboratories in addition to national and international delegations. During FY 2016 to FY 2020, CNM hosted 362 tours, with 29 groups representing international organizations and 20 from leading U.S. and multinational companies (e.g., Boeing, Corning, DuPont, Cabot Microelectronics, Wrigley Corp., Archer Daniels Midland, and Solvay). We also hosted visits from two Congressional delegations. One was led by Illinois representative Bill Foster and a second included members of the House Committee on Science, Space, and Technology: Representatives Weber (Texas), Lucas (Oklahoma), Lipinski (Illinois), Foster (Illinois), Hultgren (Illinois), Biggs (Arizona), Dunn (Florida), and Paul Dabbar, Under Secretary of Energy for Science, among others. In October 2019, we welcomed Michael Kratsios, the Chief Technology Officer of the United States. In October 2020, we hosted a visit of DOE Deputy Secretary Mark Menezes, DOE Office of Science Director Christopher Fall, and Assistant Secretary for the DOE Office of Energy Efficiency and Renewable Energy Daniel Simmons. This level of interest showcases the success of the NSRC model, which centers on our scientists and users, our cutting-edge instrumentation, and our goal of supporting a culture of cooperation and shared learning.

3.1. User Program and New Capabilities

The objective of the CNM user program is to provide the user community with access to equipment, facilities, and expertise supporting CNM's overall focus on nanoscale materials. CNM accommodates requests in three Calls-for-Proposal cycles per year. The deadlines coincide with those for the APS to maximize convenience and efficiency for overlapping user communities. User time is allocated through a proposal submission and review process in which CNM principal investigator staff, management, and external reviewers all have key roles regarding feasibility, scheduling, and scientific merit. The goal is to operate a process that is open and 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, as follows.

(i) Scientific themes: The needs of our three scientific themes first and foremost dictate all of our prioritization directions. Discussions with our Scientific Advisory Committee, our User Executive Committee, and science strategy discussions during CNM's annual strategic retreat further inform this prioritization.

(ii) Staffing needs: Needs are brought up by discussions with Group Leaders and staff scientists through a variety of means that include division-wide meetings every week, in addition to formal management team meetings. These discussions update and inform a regular list of desired capabilities that we maintain and which are dictated by our thematic science.

(iii) User and strategic needs: Emerging areas of research in the nanoscience community as defined by national research agency funding directions and strategic documents (for instance, the Office of Science Basic Research Needs Workshops and Roundtables) provide an indication of future user needs. Feedback from an annual user survey administered at the end of each proposal project is another mechanism that we use.

Based on a combination of these inputs, the Leadership Team (consisting of group leaders and division managers) deliberates to arrive at a rolling list of resources needed for future equipment capability.

Currently, CNM houses comprehensive capabilities in cleanroom-based nanofabrication; synthesis; electron, X-ray, and scanning tunneling microscopies; nanophotonics; and computational materials science. Supported by 59 scientific and other staff (including operations and administrative staff), CNM contributes to the research of approximately 600 worldwide users annually, pushes the boundaries of nanoscience research (over 300 publications with users annually), and invests in new equipment (over $2.5 million annually) to continuously upgrade our scientific capabilities.

In the next five years, we will equip CNM with unique experimental capabilities that differentiate us from other user facilities. They will be systematized into dedicated laboratories for easy access of our users to the cluster of tools designed to address current and future scientific opportunities and translational research. Below, we selectively highlight some of the new, major capabilities that we are acquiring in this timeframe.

3.2. Unique Capabilities

Quantum Information Science Capabilities

For the past several years, the CNM has added several new tools focusing on QIS research, dramatically impacting our activities within the Quantum Materials and Sensing 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. In order to attract a broad range of users and collaborators, CNM is setting 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. Collectively, these systems will enable studying ultrafast quantum dynamics, single-molecule imaging and sensing, and single-atom/molecule electron-spin-based QIS research.

We have also developed strong quantum entanglement and transduction (QET) capabilities. These are a comprehensive suite of user tools being developed for the study of quantum optics and hybrid quantum networks linking photons, spins, and magnons. 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. Finally, an adiabatic demagnetization refrigerator has recently been installed. The tool provides slightly higher temperatures (tens of mK) than a dilution refrigerator, but with faster cool-down times. The tool will be equipped with microwave spectroscopy capabilities and magnetic field capabilities to manipulate spin and is designed to probe quantum transduction processes.

Synchrotron X-ray Scanning Tunneling Microscopy (SX-STM/XTIP Beamline) Capability

Tying into our Quantum Materials and Sensing theme, this capability provides CNM with a unique and powerful angle at addressing one of the most important emerging scientific challenges in the nanosciences today: How can we sense at the single atom and single molecule level with high fidelity? We (with the APS) have recently completed the first user-dedicated SX-STM beamline (called XTIP) in the world. This provides CNM users with a unique tool, not available elsewhere, that combines the STM's atomic imaging power with the spectroscopic abilities of high-brightness, high-coherence X-ray science. The SX-STM enables characterization of elemental, chemical, and magnetic contrast at the atomic level. The XTIP beamline had first light in August 2019, and many user groups have begun to access the tool.

Ultrafast Electron Microscopy (UEM) Laboratory

The UEM forms a centerpiece for CNM's EXM group. It was installed in spring 2019 and is the first user facility for UEM within the NSRCs. Initial beta users are working with the tool now, and in early calendar year 2021 the UEM will become part of our regular user science program. 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 (TEM), lasers, detectors, and column integration. The system, as deployed, will enable observing dynamic reversible processes in events that are optically triggered (via laser excitation). The CNM UEM offers unique differentiating capabilities to the other functional UEM(s) in the U.S. 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 machine learning approaches for multi-modal multi-platform data synthesis.

Artificial Intelligence for Materials Science Capability

CNM has set forth a comprehensive software and hardware upgrade plan, which leverages recent advances in artificial intelligence to accelerate our computational materials science capabilities. The upgrades include developing user-friendly tools and capabilities and the ability to process large volumes of data effectively. These are highlighted 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 2020, we have a beta version of BLAST available to expert users. We have also built a GUI and are currently carrying out GUI integration with the backend. We expect to offer BLAST with GUI to general CNM users in FY2021. FANTASTX will have a beta version available by March 2021.

Carbon Cluster Upgrade

The CNM is investing strongly in our Carbon Computer Cluster at CNM to handle all problems associated with experimental data analysis and theoretical modeling, with additional capabilities for handling artificial intelligence problems. Built upon our existing cluster (Carbon), we are targeting 240 CPU (central processing unit)-only nodes and 40 GPU (graphics processing unit)-oriented nodes, each with two data center-class GPUs, all connected over a high-speed InfiniBand director switch and an in-cluster 2-PB storage system. Overall, the planned upgrades will triple the cluster's current compute capacity to 200 teraFLOPS on CPUs and will add 10 petaFLOPS of nominal GPU deep learning capacity. GPUs are natively suited for processing image data and certain machine learning algorithms, whereas CPUs can be used for all types of modeling.

Access to the Aurora Exascale Computer at Argonne

Aurora, the world's first exascale computer, will be deployed at Argonne in 2021 and will feature several technological innovations, including uniform high-performance memory and a revolutionary I/O system to support new types of workloads, including those relevant for data-focused image analysis and deep learning applications. It is worth noting that programming techniques already in use on CNM's current systems (such as Carbon) can be applied directly to Aurora. Aurora will have 10,000 nodes, 60,000 accelerators, > 10 PB RAM, and > 10 TB/s I/O. CNM, in collaboration with the ALCF, will serve as a gateway for nanoscience users to access Aurora.

Access to Cerebras Deep Learning Accelerator

We will take full advantage of the specialized hardware upgrades at the ALCF geared toward accelerating learning tasks. Cerebras is one such multicore engine that was deployed at the ALCF in early FY 2020. Artificial intelligence (AI)-focused architectures, such as those employed in Cerebras, pack half a million compute cores in a single node and enable massively parallel tasks involving matrix operations. This structural design is at the heart of deep learning tasks of interest to the nanosciences, such as molecular modeling, image manipulation, and inverse design. Cerebras is expected to be 1,000 times faster than CPUs and 100 times faster than current GPUs. Working with the ALCF, CNM scientists will collaborate on developing some of the first deep learning capabilities for ultra-large dataset-based materials science problems with this new--generation machine. Going forward, we anticipate that these capabilities will be available to our users.

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 TCF 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. Throughout 2020–2022, we will add several new capabilities that will allow us to: (i) carry out in-situ transmission electron microscopy of tribological interface and changes upon loading; (ii) conduct, through a scanning probe microscope-based nanotribological system, imaging of nanoscale wear tracks and determination of the nanomechanical properties of the tribolayer formed with great detail; and (iii) assess the wear/friction behavior of two-dimensional (2D) materials and nanomaterials at elevated temperatures (~500°C), uncovering the detailed wear/friction behaviors of these materials that are unknown today. Combining these new 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 ft^2 to 18,000 ft^2. CNM users have full access to the expanded portion of the cleanroom. Going forward, in agreement with Argonne management, the additional space will be used to house both CNM and non-CNM tools, and CNM will be responsible for managing 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.

3.3. A Brief Description of Accomplished and Proposed Research

In the following section we describe our specific strategic plans for each of the three themes articulated earlier. We will describe specific projects to highlight the overarching goal of each theme. It is not our intent to comprehensively list all the projects being carried out within CNM. We also indicate how the five different groups interact and engage to accomplish the objectives of the themes. Finally, our equipment purchase plans required to accomplish the work are presented.

Theme I—Quantum Materials and Sensing

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. We address materials for QIS that we categorize into two kinds. The first deals with solid-state systems that involve the creation and manipulation of coherent quantum of information for sensing, computing, or communication. Single-photon emitters and optically active spin systems have emerged as powerful platforms for this, because they can be initialized, manipulated, and read out remotely with light; they can store quantum information in the long-lived spin degree-of-freedom; and they can serve as sensitive sensors at nanometer length scales. These systems can take the physical form of defects or dopants in a host matrix, or of semiconducting particles, which are nanostructured for quantum confinement. Either way, 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. We hope—through our own science and the user science that CNM enables—to further the fundamental science leading to the creation, storage, manipulation, and entanglement of quanta of information using these nanoscale solid-state systems. The studies include the fundamentals of spin, single-photon, phonon, and magnon dynamics; sub-wavelength light localization; and topological materials, as well as the creation and manipulation of dopants and defects in materials for quantum coherence and entanglement. These phenomena comprise the underlying science for any practical quantum system (computing, sensing, or communication) and the building blocks for qubit transduction schemes, quantum memories, and information transport (Figure 3-1).

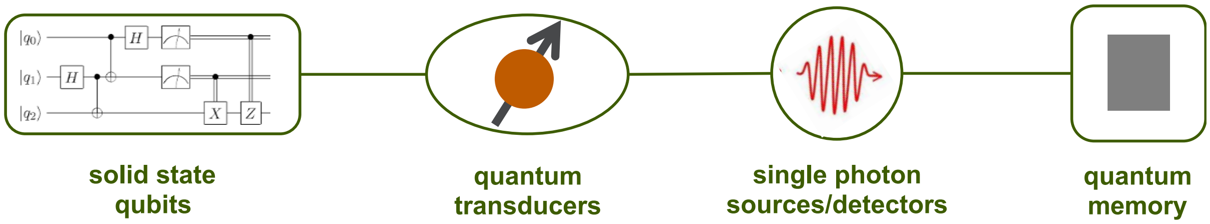


Figure 3-1: Schematic presentation of the building blocks for qubit transduction schemes, quantum memories, and information transport.

The second kind deals with sensing at the single-atom/molecule level using quantum mechanics to maximize the information that we can obtain, though not necessarily via quantum systems that are coherent or entangled. Atomic resolution sensing is also gaining vast interest in the nanoscale research community. CNM's involvement in this area goes back five-plus years, where we combine the strengths of the scanning tunneling microscope with synchrotron X-ray excitation of materials in a single tool and technique (SX-STM), now operational at the XTIP beamline in collaboration with the APS. It builds on our traditional strength in near field microscopy and X-ray science.

In the following discussion, we highlight details about two broad areas of our research focus in this theme: (1) next-generation quantum emitters and spin-based qubit systems for QIS and (2) sensing at the single-atom/molecule level.

To address these areas, we have added the participation and new skills of five scientist hires. They build upon established materials and characterization strengths that are unique to CNM, thus differentiating our capabilities to users. For instance, the optical and spin physics work derives from and builds upon the strong nanophotonics presence that CNM traditionally has had. Designing and building single-photon sources and nonlinear resonators rely upon CNM's colloidal synthesis and nanofabrication capabilities. The research to study strain effects in qubits derives from CNM's unique HXN capability, which is made possible by the presence of the APS synchrotron facility. Our work on QIS at surfaces centers around our extensive capabilities in ultrahigh vacuum (UHV) scanning probe spectroscopy.

Next-generation quantum emitters and spin-based qubit systems

We believe that solid-state qubits are of rapidly increasing interest in the scientific community (and to future users) because of their anticipated scalability and the rich physics they enable. Here, we explore the underlying materials science and physics of solid-state qubits based upon spin and optical photons, and the transduction of information coherently between different solid-state qubit systems. We envision a compact solid-state quantum information system as one, where coherent excitations are transducted between solid-state spin qubits operating at a circuit level and single photons, which then carry the information over longer distances. This research thrust thus examines the science of deterministic single-photon sources, spin-based microwave qubits, and quantum transduction between the two.

Optical photons and their long coherence times make them well suited for use in quantum logic operations and quantum sensing, as well as in long-distance quantum information transfer. Our research goal towards compact, deterministic "on-demand" single-photon sources builds upon our decade-long experience in the colloidal synthesis of engineered semiconductor nanomaterials and optical physics (Figure 3-2) and our recent work (*ACS Nano* **11**, 9119 [2017]; *Nano Lett*. **18**, 4647 [2018]; *Nat. Comm.* **10**, 3253 [2019]; *Nano Lett*. 20, 5866 [2020]; *Adv. Funct. Mater.* 30, 1904179 [2020]).

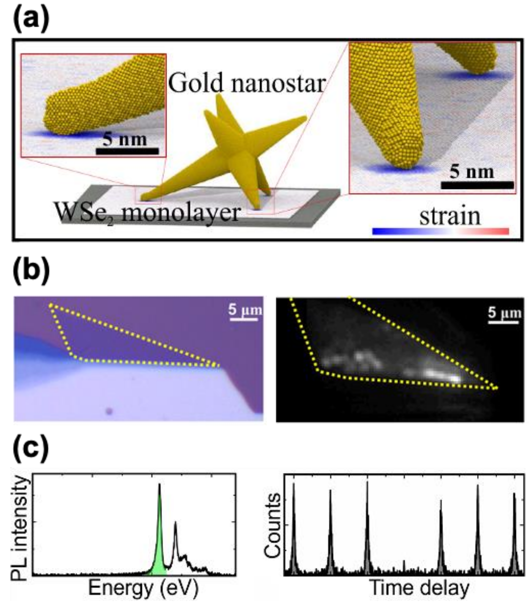


Figure 3-2: (a) Schematic of strains induced by gold-nanostars on WSe_2 monolayers. (b) Optical micrograph (left) and photoluminescence image (right) of a WSe_2 monolayer. The bright spots in the right image corresponds to single-photon sources. (c) Sharp emission spectrum (left) and photon antibunching from the single-photon emitters (L. Peng at al., *Nano Lett*. **20**, 5866 [2020]).

There is widespread interest in solid-state spin-based qubits. Our planned activities cover approaches that offer superior quantum environments for long coherence times, scalability based on chip technologies, and controllable interaction via integration with platforms such as silicon photonics. Among these approaches, we will pursue noble element quantum solids, such as He-4 and Ne-20, for single-electron spin qubits, because of their ultralow defect counts, zero atomic spins, and soft atomic bonds. Using our skills in nanofabrication, we will systematically develop a new on-chip qubit platform based on the quantum solids filled in patterned microfluidic channels and integrated with radiofrequency traps and single-electron devices. In a second approach we are exploring embedded atom qubits (within dielectric heterostructures) based on rare earth elements, where the shielded 4f shell levels offer long-lived, protected states that are optically addressable. Both approaches are highly scalable and compatible with silicon wafer environments. To date, work on spin qubits has centered on defects or dopants buried deep inside near-perfect crystals. However, this significantly limits their potential impact, curtailing the ability to control these systems. In a third approach—leveraging our years of experience in 2D materials we are developing capabilities to explore optical and spin coherence near or at surfaces on their native length scale by utilizing UHV scanning probed microscopies (SPMs) coupled with integrated, high numerical aperture optics (Figure 3-3). Probing near-surface single quantum emitters with atomic-scale control in 2D materials will open up new opportunities for the user community.

We are and will continue to use our deep expertise in X-ray and electron microscopy to understand the microstructural and chemical basis of coherent quantum information flow. For example, the manipulation of strain near isolated point defects and engineered structures provides a route to controlling a solid-state qubit environment without introducing stray electromagnetic fields. The degree and nature of strain coupling to local properties, such as energy level degeneracy, are poorly understood. Using CNM's unique HXN capability at the APS, we have recently developed a technique of three-dimensional (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.

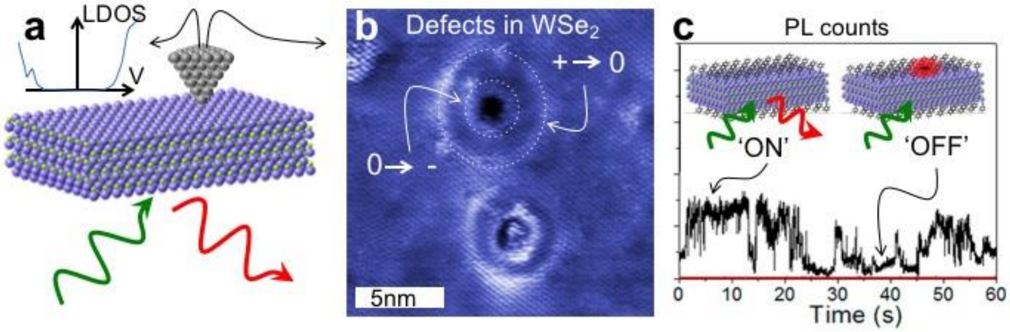


Figure 3-3: (a) Schematic of SPM used to correlate the optical properties with local electronic structure (inset); (b) STM image of WSe_2 showing rings associated with changing of the defect charge state (V_B = -1.17 V, I_t = 700 pA); and (c) time trace showing the "blinking" of photoluminescence (PL) emission (adapted from Tessier et al., *ACS Nano* **6**, 6751 [2012]).

We now turn to quantum transduction. Quantum information in different excitations or formats may operate in different frequency regimes: microwave photon, optical photon, electron spin, nuclear spin, etc. The science of quantum transduction—studying how quantum information can be coherently transferred from one format to another without converting to classical information—and of building nanoscale quantum transducers is thus an important topic of interest. We have begun our research in this area with hybrid magnonic systems, where microwave photons, optical photons, and mechanical phonons coexist with collective spin excitations (i.e., magnons) in these systems with very low losses. We will first take advantage of the nanofabrication capability at CNM to bring conventional magnonics to the nanoscale and study the fundamental physics of hybrid magnonics in the quantum regime. Following this effort, we wish to study the integration of different qubits to explore the principle of coherent information exchange within quantum networks at small scales (Figure 3-4).

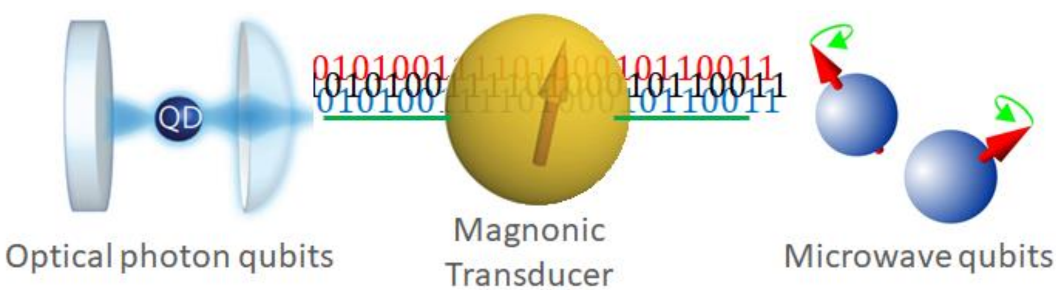


Figure 3-4: Magnonic quantum transductor and a simplified distributed quantum network for qubit and protocol testing.

Our experimental systems used for these studies, which broadly enable characterization of magnetic, optical, and electronic properties of spin-based and magnonic systems, are available as user tools to serve the large QIS community for studying distributed quantum networks. These tools will allow users to manipulate and interconnect microwave qubits and optical photon qubits to enable experimental research on new qubits and qubit networks.

Theory and simulation are essential both to enable the experimental QIS outlined in this plan and drive new experiments and directions. The in-house expertise of the TMG group in electronic structure, electrodynamics, and cavity quantum electrodynamics (cQED) makes CNM researchers particularly well suited for carrying out such work. For example, we will carry out cQED calculations to enable the generation and detection of entangled photons and understand how efficient transduction of quantum information can be achieved. We also envision more theory-driven efforts in understanding and predicting entanglement-facilitated phenomena in ensembles of qubits (e.g., quantum dots or nitrogen-vacancy centers).

Sensing at the single-atom/molecule level using the SX-STM

A second aspect of this theme deals with using quantum mechanics for single-atom/molecule sensing and incorporates our ongoing work on the SX-STM. The SX-STM has been incorporated into the new XTIP beamline at the APS and began user operations in August 2019. By combining local scanning probe imaging and tunneling spectroscopy methods with a variety of synchrotron X-ray methods, this system will attain an unparalleled performance for investigating materials surfaces and interfaces with simultaneous elemental, chemical, magnetic, and topological contrast, with the spatial resolution potentially down to the atomic and molecular scales. To date, the SX-STM system has achieved a spatial resolution of 2 nm lateral and 0.2 nm vertical at room temperature. Ultimately, we hope this technique enables us to identify single atoms and image their chemical and magnetic signatures.

Theme II—Manipulating Nanoscale Interactions

A central motif here is to study and control the forces, electromagnetic interactions, and energy dissipation between nanoscale constituents at interaction lengths that vary from the atomic scale (~0.1 nm) to distant (~100 nm). These interactions can be collective and dissipative, making it challenging to predict and control them. This is the case in a large variety of nanoscale systems, such as the nonlinear dynamics of nano-electromechanical systems (NEMS) and metasurfaces (10–100 nm), the fundamentals of friction at the nanoscale (1–100 nm), the molecular dynamics simulations of materials (1–10 nm), and the synthesis of heterogeneous materials (0.1–100 nm). This common motif ties together the major planned research thrusts at CNM belonging to Theme II: Computational Molecular Dynamics and the three experimental areas that these theoretical studies inform: the Science of Tribology and Superlubricity at the Nanoscale, the Science of Metasurface Engineering, and the Synthesis of Nanomaterials Across Scales. These thrusts feed into one another, with close interaction between the subject matter experts. For instance, within CNM, collaboration between the computational molecular dynamics experts with the experimentalists studying nanoscale tribology led to the discovery of scalable superlubricity (near zero friction) conditions (*Science* **6239**, 1118 [2015]). The synthesis inputs led to the nanoscale "ball bearing" like moieties that resulted in superlubricity conditions (*Nature Comm.* **9**, 1164 [2018]; *Appl. Phys. Lett.* **115**, 103103 [2019]). Our strategy for this theme relies heavily upon CNM's extensive NEMS and nanofabrication expertise and our traditional strengths in nanomaterials synthesis, optical physics, and computational materials design.

Our research on computational molecular dynamics is informed by artificial intelligence techniques, and feeds into all three of our science research themes by providing broad materials discovery and materials design guidance. Here, CNM's goal has been to apply machine learning and data science approaches in concert with first principles physics and/or experimental data, to develop a suite of significantly more accurate (compared to what is available today), yet computationally efficient approaches for simulating the interaction between atoms for molecular dynamics calculations. This work builds upon remarkably promising results obtained by us over the past 2.5 years (see, for instance, *Nature Comm*. **10**(1), 379 [2019]). Our efforts over the next five years will include the development of a set of user tools for molecular dynamics simulations of materials informed by artificial intelligence. The use of artificial intelligence for the physical sciences is of great interest to the scientific community and also has emerged as a focal point of emphasis for DOE's Office of Science as described in the sections above. We, therefore, anticipate significant user interest in this area over the next five years.

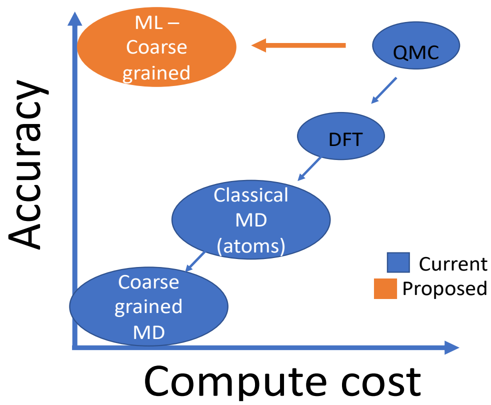


Figure 3-5: Our machine learning (ML) framework combining the speed of coarse-grained potentials with the accuracy of quantum monte carlo (QMC) simulations. This treatment will enable high-fidelity, long-timescale simulations of multimillion-molecule systems to probe the nucleation and growth phenomena in hierarchical materials.

We will explore new means of determining flexible force fields for large-scale molecular dynamics simulations capable of describing reactive catalytic processes, disorder, and phase transformation much more accurately and efficiently than is possible today. We plan to do so by leveraging active learning strategies that we have already developed successfully to sample computationally expensive but accurate training data efficiently. Such strategies can train models against much sparser datasets compared to those in conventional training procedures.

Our end goal is to design inexpensive, yet accurate machine learning molecular models (Figure 3-5) that will be available to our users and will accelerate materials design and discovery in at least two ways. First, they will be combined with artificial intelligence-based decision tree approaches to explore the structural phase space and perform "inverse design" to predict optimal structures for user-defined target properties. Second, they will be combined with computer vision and deep learning approaches to build and train deep (convolutional) neural network classifiers for supporting microscopy experiments (see the description of Theme III, Nanoscale Dynamics, for more details).

Synthesis of nanomaterials across scales represents a broad, traditional area of strength for CNM and influences research in all of our three scientific themes. Here, we have made significant progress over the past decade in the control of zero-, one-, and two-dimensional materials synthesis using a variety of colloidal and solution chemistry, biochemical, and vacuum deposition methods. We will continue our efforts in this direction of synthesis, and over the next five years, we will increasingly use these capabilities to focus on integration and functionality. Examples include the incorporation of plasmonic nanostructures for metasurface engineered flat lenses (discussed below), the synthesis of hybrid nanomaterials as solid lubricants for superlubricity applications, and the synthesis of single-photon emitting quantum materials.

An additional area of focus is that of synthesizing, understanding, and utilizing the interactions of inorganic nanoparticles with biological or bioinspired materials for applications in optical energy conversion and sensing. An example is the use of cell-free synthetic biology approaches to create "nano-bio" composites of synthetic purple membrane "proton pumps" in concert with TiO_2 and Pt nanoparticles for photocatalytic hydrogen production (*ACS Nano* **11**, 6739 [2017]; *Angew. Chemie* **58**, 1 [2019]; US Patent 10,220,378). We further plan to develop our nano-bio expertise for highly specific and sensitive nanostructured sensors, ultimately to be used in concert with 2D waveguide arrays for on-chip sensing in collaboration with the Quantum Materials and Sensing theme.

In another area, we turn our attention to biofilms. Bacterial biofilms are the prevailing microbial lifestyle on earth and play a critical role in many areas relevant to energy research. However, the specific mechanisms of biofilm decision-making, where film morphologies and function depend upon the collective signaling between its microbial constituents, are not well understood. In collaboration with our colleagues in Argonne's Biosciences Division, we have initiated an exploratory study to combine systems biology and dynamic optical imaging to unravel the underlying principles of biofilm decision-making. Our approach relies upon the fluorescent tagging of chemical messengers universally conserved in all bacteria. Guided by these principles, we will study the underlying science for engineering artificial structures (protocells, inorganic capsules, etc.) capable of performing environmentally beneficial functions (for instance, corrosion protection layers or self-healing protective films). Through this effort, we also hope to increasingly attract users from the biological community.

Our research on molecular simulations and synthesis contributes to our efforts on the science of tribology and superlubricity at the nanoscale. CNM's unique research and direction harnesses 0D and 2D nanomaterials and carries out discovery science in solid-state lubricants for superlubricity (state of zero friction) under realistic conditions. As a collaboration between nanomaterials synthesis experts, molecular dynamics experts, and experimentalists working on nanoscale tribology, it has enabled CNM to carve out a unique niche in this space. Obtaining a fundamental understanding of the atomistic-scale dynamical processes at tribo-interfaces is crucial for the design of functional lubricants. Our recent experimental studies over the past three years have shown that 2D materials (including graphene, MoS_2, and hexagonal-BN), when combined with nanoscale diamond particles, undergo tribochemical reactions at the nanoscale, leading to formation of onion-like-carbon "bearing" structures at the tribological contact during the sliding process. This yields superlubricity at macroscale. We will build on these exciting results over the next five years in broadly developing the field of superlubricity at the macroscale using nanomaterials engineering. Our studies will include the visualization of tribochemical modifications in real time at the tribological contact down to the atomic level to better understand the mechanism(s) of superlubricity. It will also include exploring the materials phase space to identify other 2D materials in different environmental conditions (in air, in vacuum, and at elevated temperatures of 200–400°C).

Our research on superlubricity has received particular attention from industry. We have been successful in receiving recent funding from DOE under TCF grants in collaboration with John Crane, Inc., and Magna. In these efforts we are developing superlubricity solid lubricants based on 2D materials and other nanomaterials for dry gas seal and metal stamping applications.

Our research under this theme rounds out with our efforts in the science of metasurface engineering, where we harness collective interactions at the ~10-nm length scale to study and create metasurface and NEMS-based miniaturized optical systems. All bodies are surrounded by fluctuating electromagnetic fields due to thermal and quantum fluctuations of the charge and current density at the surface of the bodies. Immediately outside the bodies, this electromagnetic field exists partly in the form of propagating electromagnetic waves and partly in the form of evanescent waves that decay exponentially with distance away from the body's surface. In this research theme, we intend to implement reliable methods to probe, control, and manipulate nanostructures by controlling these near-field forces.

Nanostructured surfaces, or metasurfaces, represent a unique system from which to harvest nanoscale near-field interactions. Metasurface-based optical elements enable wave-front engineering by locally controlling the properties (amplitude, phase, etc.) of the incident illumination. They hold great potential to promote a new generation of "ultra-flat" lenses and thin optical systems for imaging and sensing. At CNM we are exploring ultrathin (thinner than wavelength) metasurfaces based on dielectric nanoresonators. Using a machine learning-based inverse design strategy to guide experiments, we have been able to demonstrate the thinnest and highest transmissive metalenses reported to date. This research will continue over the next few years to take full advantage of the strong interactions between nanoresonators to understand and implement novel metasurfaces for manipulation of visible light and novel sensing platforms.

Furthermore, by integrating arrays of optical nanoscale resonators onto NEMS devices, we intend to develop reconfigurable devices capable of delivering optical properties on demand, a concept we recently demonstrated (*Appl. Phys. Lett. Photonics* **3**(2), 021302 [2018]; see Figure 3-6). Over the next few years, this concept will be scaled up to the design of optical systems with apertures as large as 1 cm. Our NEMS-based metasurface engineering and nanofabrication activity has also drawn interest from companies such as Frore Systems, a micromechanical system (MEMS)-based Silicon Valley startup. We will collaborate with them over the next few years.

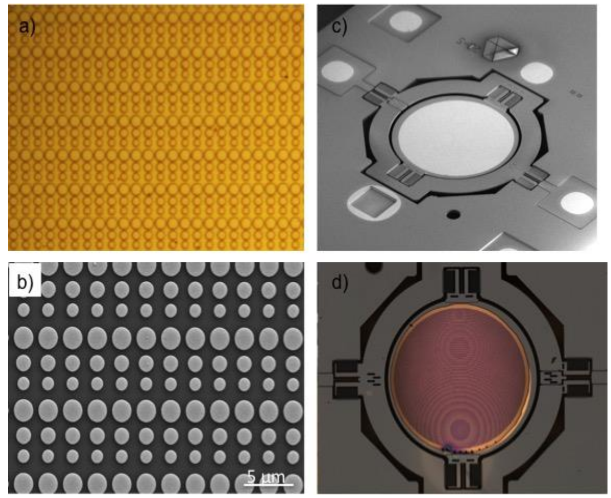


Figure 3-6: Example of integrating metallic metasurfaces into MEMS scanners. (a,b) Optical and SEM image of a plasmonic flat lens designed to focus infrared light at 45° of the incident angle. The lenses were integrated into a 2D MEMS scanner used for pattern generation: MEMS scanner (c) before and (d) after metasurface integration.

Theme III—Nanoscale Dynamics

Today, there is significant interest in interrogating, visualizing, and understanding time-dependent phenomena in materials at the nanoscale at ultra-short (femto- to nanosecond) time scales. This includes understanding the evolution of metastable materials and lattice phase changes, non-equilibrium mechanical response, 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 believe we have, therefore, made a timely decision to identify nanoscale dynamics as a key theme for staff and user science at CNM. 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, such as catalysis and soft matter. The theme supports and closely affects both Themes I and II.

Our nanoscale dynamics research rests upon three major experimental approaches. The first continues to build upon our strong, productive, and traditional efforts in ultrafast optical physics, which we will expand and broaden, for example, into spatially resolved ultrafast spectroscopy and imaging. The second develops a major new initiative, UEM, the rationale for which we describe below. The third targets time-resolved HXN imaging that will be enabled by the high “per-bunch” brightness of the synchrotron beam following the APS Upgrade. This approach builds upon CNM’s extensive expertise in HXN microscopy over the past several years. We will use these three approaches in close concert, as well as collaborating with CNM’s theory group.

Our ultrafast optical physics research will revolve around two techniques: ultrafast optical microscopy (UOM) and Fourier plane transient absorption microscopy (FPTAM). CNM currently offers an encompassing range of spectroscopic capabilities with single-picosecond time resolution—however, we lack high spatial resolution spectroscopic methods. To overcome this shortcoming, our aim in the coming years is to develop the UOM with both high temporal and spatial resolution, as well as the FPTAM, each of which complements our efforts with UEM. They will be used to address two important areas in the transient response of materials: effects that are triggered inhomogeneously and the role of electron-phonon dynamics in transient excitations of materials and thermal dissipation.

Multiple classes of materials problems and sample types are prompting 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 Mater*. **14**(5), 484–489 [2015]). Often such inhomogeneities play key roles in the local nucleation and triggering of events, such as in carrier trapping, energy funneling to defect sites, or phase transitions, such as metal-to-insulator transitions. The UOM offers the spatial and temporal resolution ideal for such studies. Characterizing the time scale and channels into which energy flows upon impulsive excitation is fundamental to a wide range of nonequilibrium phenomena. However, discerning mechanical motion such as phonon generation and thermal dissipation can be challenging to evaluate, given that electron–phonon scattering can occur on the femtosecond to picosecond time scale (*Nature Comm.* **8**, 986 [2017]). This type of scattering limits the tools capable of optically measuring the population decay of energetic carriers. We aim to overcome this challenge with the development of the FPTAM, as detailed in Figure 3-7.

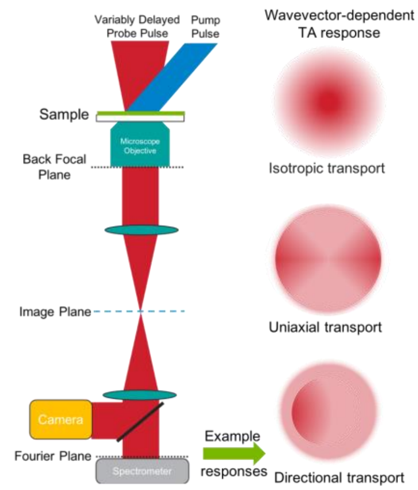


Figure 3-7: Schematic of the proposed FPTAM. Signal collection that images the objective Fourier plane offers wavevector-dependent absorption that can be collected as a function of probe delay, such that time-dependent wavevector evolution of electron–phonon coupling and phonon propagation processes is measurable.

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. We expect that FPTAM will play a critical new role in visualizing these processes in various crystalline materials by revealing changes in the anisotropy of photoexcitation as a function of time. Success here will yield an unprecedented route to spatially and spectroscopically characterize the temporal and spatial evolution of electron–phonon coupling in varied material systems.

The experimental effort will be strongly coupled to our theoretical effort. Concomitantly, we will perform theoretical modeling of nonequilibrium electron–phonon dynamics, using a combination of many-body perturbative, Boltzmann transport equation, and first-principles molecular dynamics approaches (Figure 3--8). In particular, we aim to understand how electron–phonon dynamics are impacted by nanoscale heterogeneity, anisotropy, interfaces, and electron/phonon localization.

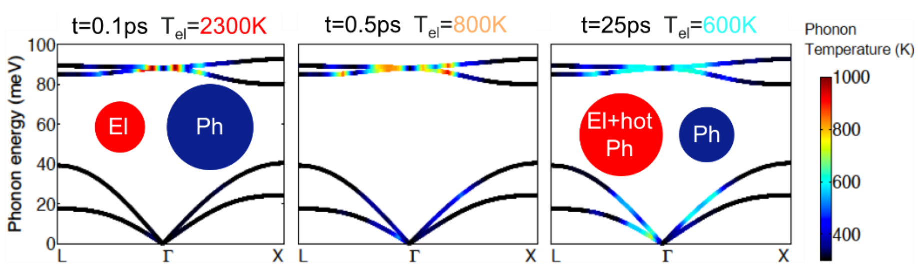


Figure 3-8: Ab initio modeling of electron–phonon dynamics revealing nonequilibrium distribution. CNM will build upon this capability in coming years.

Our UEM research will center around an electron column-based UEM (Figure 3-9) that was recently installed. It is currently available to expert β-users and will become available to the general user community in early 2021. It combines a state-of-the-art, high-repetition-rate, tunable femtosecond laser with a synchronous laser-pumped, pulsed TEM that is outfitted with high-sensitivity cameras and electron energy filtering. This tool, which we have carefully designed and have rapidly brought online, opens the door to an otherwise prohibitive, specialized technique both for CNM staff and the broader user community. The UEM permits the means to evaluate sample 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. It represents a key experimental method that can deliver insights on ultrafast structural and chemical changes to a wide range of systems. However, to date it has been available only to a few research groups that have specialized in technique development. There are many areas of nanoscience where the UEM can be highly valuable in advancing our understanding of transient processes, such as in exciton localization, short-lived metastable phases, photo-induced segregation, dynamics in topological materials, plasmonic systems, molecular motors, and magnetic fluctuations, to name a few.

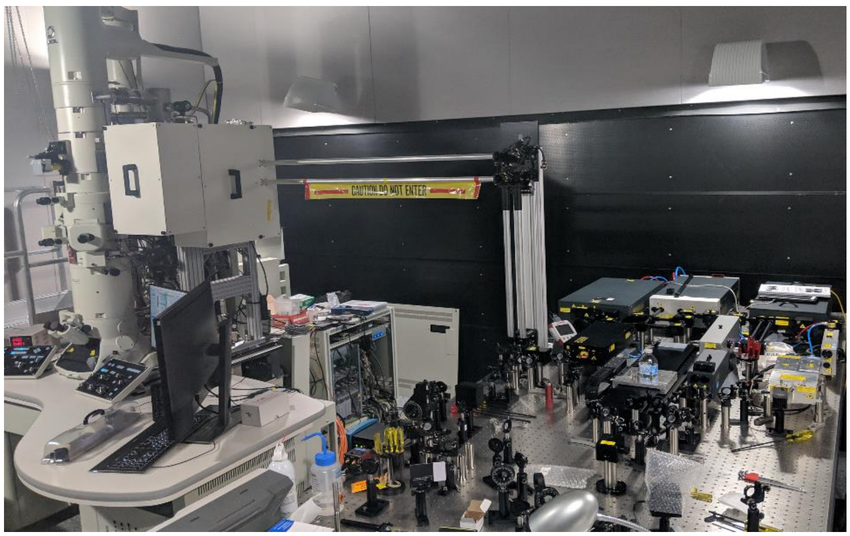


Figure 3-9: The Ultrafast Electron Microscope. It features a femtosecond tunable pump laser, multiple routes to produce the pulsed electron beam, and electron energy filtering in a state-of-the-art building specific to electron microscopy.

Initially, reversible processes that occur in response to optical triggering will be studied in real and momentum space via stroboscopic UEM that delivers 1–1000 electrons per pulse (depending on time-resolution needs). Transient crystallinity changes and alteration in charge carrier densities will be accessible with diffraction and electron energy loss methods.

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. Combined with ultrafast probing, this will permit insights into non-equilibrium phenomena of electric field and strain. In particular, structural distortions that exist upon formation and disturbance of quantum fluids will be targeted, as will in-operando nano-enabled transistors, memories, NEMS behavior, and the response of microstructure to ultra-high strain rates.

We have received strong interest from potential users. We held a UEM workshop in April 2019 at Argonne with over 40 attendees, where approximately 16 UEM experts presented invited talks from throughout the United States and abroad. Roughly half of the attendees were external. The internal half of attendees spanned six different divisions/directorates within Argonne, highlighting the versatility of science that will be available using this capability. The purpose of the workshop was to build a user community, identify ultrafast science needs, and identify the additional technique developments that would be necessary to meet those science needs.

CNM is planning to upgrade HXN's capabilities 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. By synchronizing stroboscopic scanning X-ray diffraction microscopy 3D visualization to 100-ps synchrotron X-ray pulses, our goal is to create a dynamic diffraction 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 acoustic or optical dynamic stimulation of defects in materials. This capability can 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 rendered 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.

4. Synergies with Other DOE User Facilities at Argonne

CNM leverages its science and capabilities with the strengths of the other BES user facilities co-located at Argonne. Examples of such synergies are provided below.

4.1. Hard X-ray Nanoprobe (HXN) Facility

CNM's HXN facility, located at Sector 26 of the APS, was jointly built and operated by CNM and APS. It is the only dedicated X-ray microscopy facility within the portfolios of the nation's five NSRCs, and its nanoscale imaging capabilities are best-in-class for experiments involving dynamic measurements of materials. CNM directs the scientific program, manages the operations, and provides the majority of the funding for the HXN. APS provides scientific and technical support to the HXN through an in-kind effort contribution. Experimental beam time at the HXN is allocated on a 75%-25% basis between CNM and APS. Proposals for beam time may be submitted either through the APS or CNM proposal submission portals. As part of our collaboration with APS, we are adapting the microscope infrastructure to deliver transformative microscopy of dynamic systems and thermal transport, harnessing the diffraction-limited storage ring of the APS Upgrade.

4.2. Dedicated Beamline for Synchrotron X-ray Scanning Tunneling Microscopy (XTIP)

A successful example of the CNM synergy with APS is the recent development of the world's first dedicated SX-STM beamline, XTIP, at the APS. The XTIP beamline became operational in August 2019 at APS Sector 4, and takes full advantage of the brightness and polarization control of the undulator source there. In FY20, 12 separate user groups accessed the XTIP beamline and we expect demand to continue and growth of the SX-STM user community. The coming upgrade of the APS to create a brighter, more coherent light source is expected to continue to improve the range of experiments possible with the SX-STM technique.

4.3. MEMS X-ray Pulse Selector

Recent collaboration between CNM and APS also led to work that resulted in a MEMS X-ray pulse selector, a new class of devices for controlling sub-nanosecond timing of X-ray delivery. Shrinking of X-ray optics to the microscale using MEMS technology created an opportunity for developing ultrafast devices that reflect X-rays at precise times and specific angles. Recent experiments demonstrate that these devices can achieve sub-nanosecond gating windows (~300 ps) , ~2 orders of magnitude better than the typically used mechanical choppers. This work is expected to lead to compact, sophisticated X-ray optical approaches for studying the structure and dynamics of matter at atomic length and ultrafast timescales and lay the groundwork for the development of a suite of X-ray optics (e.g., ultrafast gating devices, multiplexers, and ultrafast spectrometers/monochromaters) to facilitate experiments currently not possible at X--ray synchrotrons.

4.4. Integrated Computational Tools

CNM's TMG has strong associations with the ALCF, including the DOE INCITE projects on understanding the molecular origins of climate change, reactive mesoscale simulations of tribological interfaces, mesoscale combining high-accuracy electronic structure methods to study surface reactions, and mesoscale reactive simulations of electrochemical surfaces. These projects involve employing significant computer time on some of the fastest supercomputers in the world, as well as working closely with ALCF staff members to develop and improve the performance of molecular dynamics codes (LAMMPS and NAMD) and on quantum Monte Carlo electronic structure approaches. TMG also works with members of the ALCF to develop preproposals and proposals in emerging areas such as QIS. We will develop and apply, both in simulation and on actual quantum computers such as IBM-Q (which Argonne scientists can access), quantum algorithms for finding the quantum dynamics of chemical reactions. Members of the ALCF also attend TMG's meetings.

4.5. Partnership with the Laboratory

As noted in section 3.2, Argonne has completed construction of a 6,000-ft^2 cleanroom space connected to CNM's existing cleanroom. The extension of the existing cleanroom will house prototyping, testing, and fabrication equipment to enable the advancement of nanoscale devices from the research phase to development. It will also house key synthesis and fabrication tools as part of the recently funded Q-NEXT center, a $115M National Quantum Information Research Science center. The cleanroom extension will be available to CNM users.

5. Crosscutting Research with Other Programs

5.1. Crosscutting Research with Core Research Programs at Argonne

Science and capabilities at CNM leverage core research strengths with several research programs at Argonne, listed below.

***Computational Materials*:** CNM's TMG participates in the Center for Electrochemical Energy Science (CEES, a DOE Energy Frontier Research Center); the Midwest Integrated Center for Computational Materials (MICCOM, a DOE Basic Energy Science-funded Center); SunShot Bridging Research Interactions through Collaborative Development Grants in Energy (BRIDGE, a DOE Energy Efficiency and Renewable Energy program); and a Strategic Partnership Project (SPP) with Toyota Research Institute of North America (TRINA). In CEES, we have developed computational approaches to configurational sampling for non-equilibrium electrochemical processes in high-capacity lithium-ion and beyond-lithium-ion energy storage materials, and a computational capability for modeling Raman spectra. In MICCOM, we are developing scale-bridging capabilities for modeling solid-liquid interfaces and thermal transport in nanostructured materials. In the BRIDGE project, we are developing a high throughput computational framework for sampling and evaluating grain boundaries in semiconductors. As part of the SPP with TRINA, we have developed methodology to study the electronic and thermal transport properties of metal-insulator materials. These new capabilities strengthen and expand the intellectual and scientific expertise that is available at CNM.

Photon Dynamics: Our expertise in time-resolved spectroscopy has contributed to a DOE BES ultrafast science project that aims to determine impacts of coherent phenomena on electronic processes, such as molecular motion-driven photocatalyst activation. In this project, CNM is making time-resolved optical measurements of nanomaterials that exhibit coherent vibrational motion and correlating them with electronic phenomena such as energy transfer. The results aim to connect to non-equilibrium energy flow and photocatalysis.

Quantum Materials: CNM is collaborating with a DOE BES Materials Sciences Program with the Center for Molecular Engineering (CME, a partnership between the University of Chicago and Argonne) entitled Quantum Metamaterials. The collaboration intends to establish a vibrant quantum materials and sensing research effort within Argonne and to benefit from the deep expertise that currently exists at CME on the subject. The goal is to explore the physics of quantum states and entangled states for energy-efficient information processing.

Quantum Information Science: Argonne is the lead laboratory on a National Quantum Information Science Research Center recently selected for funding entitled "Q-NEXT: Next Generation Quantum Science & Engineering". The center partnerships included 3 national labs, 10 academic institutions, and 10 companies. Q-NEXT will address one of the most prominent cross-cutting challenges facing quantum science today: manipulating and interconnecting entangled states of matter. In this effort, Q-NEXT will leverage the user science capabilities in quantum information science at the CNM, particularly in the areas of fabrication, quantum optics, X-ray nanoprobe microscopy (collaborative with the APS), and ultrafast optics.

Rare Earth Materials: CNM staff recently led and won a DOE BES Critical Materials Award for "Design, synthesis, and atomic scale characterization of rare-earth base supramolecular nanographene and nanoribbons." This work is responsive to DOE interests in basic research on rare earth elements and the unique technologies these materials enable in areas such as energy and national security.

5.2. Partnership with Users

Several partner user proposals (PUP) are in place at this time with various Argonne divisions.

Terahertz Physics*:* CNM has developed time-resolved terahertz (THz) spectroscopy consisting of an optical pump and THz probe that leverages a femtosecond amplifier in the CNM laser labs, while the APS funds the construction of a THz spectrometer. THz spectroscopy is valuable for studying a large range of condensed matter phenomena, including phase transitions in complex oxide nanomaterials and coupled spin and valley dynamics in 2D transition metal dichalcogenides. When fully complete, CNM staff and users will gain a new, cutting-edge capability for characterizing nanomaterials at THz frequencies, including THz time-domain spectroscopy with THz-pump/THz-probe and THz-pump/optical-probe, along with the currently operating optical-pump/THz-probe. These capabilities will complement newly developed THz-pump X-ray probe capability at the APS.

Superconducting Bolometers for the South Pole Telescope*:* A PUP with Argonne's High Energy Physics Division involves a research and development effort with CNM to fabricate large arrays of multi-chroic transition edge sensor (TES) bolometers for use in cosmic microwave background (CMB) experiments (Figure 5-1). The focus is on developing techniques to implement and control the lateral proximity effect and reduce two-level-system loss in superconducting microstrip at millimeter-wave frequencies. The goal is the stable and robust production of multi-chroic microstrip-coupled TES bolometer arrays across multiple 150 mm substrates. Several tools installed in the CNM cleanroom as part of this PUP are available for users (an ASML stepper, an etcher, and two AJA deposition tools).

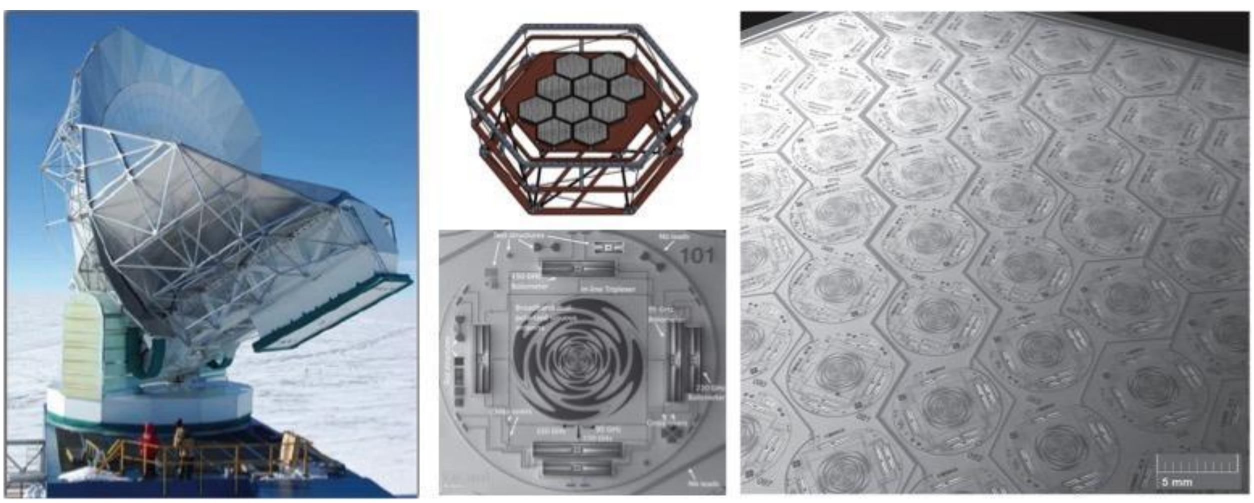


Figure 5-1: Clockwise from left: South Pole Telescope, where the next-generation CMB polarization experiments are performed; CAD drawing of the SPT-3G focal plane and support structure; SEM micrograph of a fabricated SPT-3G multichroic pixel array, including the wiring layout; and SPT-3G multi-chroic individual pixel.

Finite Element Simulations*:* This PUP with APS utilizes the high-performance computing Carbon cluster for finite element simulation. The PUP allows APS access to the CNM- licensed COMSOL finite element software for development of capabilities that can help APS to design better scientific instruments. APS enhances COMSOL capabilities by adding modules that allow APS and the CNM user community to use multi-physics simulation capabilities. Some projects include nano-positioning for X-ray optics and samples, design of an acoustic levitator to dispense nanoliter samples, design of ultra-high heat flux front-end and beamline components, design of mirror bending and focusing piezo-electric actuators with nanoscale actuation, and design of a nano-size beam analyzer.

Polarizers and Coherent Diffractive Imaging*:* A partner user proposal with APS encompasses hard X-ray polarizers and dichroic coherent diffractive imaging for development of a new capability for imaging nanomagnetic structures simultaneously with crystal lattice strains. This project advances our goals to develop dichroic coherent imaging capabilities at the CNM HXN and SX-STM programs at beamline 26-ID, and to position the Nanoprobe to take full advantage of the unprecedented hundred-fold increase in coherent flux to be provided by the APS upgrade.

5.3. Industrial Outreach

One CNM goal is to increase industrial user participation to more fully embrace nanotechnology aspects and relevance to applied technologies. Recently, CNM has successfully leveraged DOE's TCF to develop industrial partnerships. For instance, current TCF-supported technology partnerships are with Magna International and John Crane for developing nanomaterials-based solid lubricants that exhibit superlubricity, and with Boeing and Sentient Science for developing artificial intelligence-informed materials simulations. Other industrial partners have included researchers from large companies, such as Corning, Inc.; Toyota Research Institute of North America; IBM; HP; GE Global Research Center; and Applied Materials. Small business partners include Creatv Microtech; Advanced Diamond Technology; OptoNet, Inc.; Iris Lighttech (a spinoff from CNM); and Frore Systems (a Silicon Valley MEMS startup). Awareness of CNM's user capabilities within the industrial community has expanded recently to include Toyota Motor Engineering and Manufacturing North America, Inc.; Brewer Science, Inc.; several small businesses; and the integration of industrial users, such as BP and UOP, LLC. The latter are large oil companies primarily interested in catalyst development when accessing CNM. CNM's industrial users have accessed all aspects of our capabilities, including the HXN beamline, the nanofabrication facilities, various microscopy techniques, and the high-performance computing cluster. Finally, additional information on proprietary research at the CNM is available on our website (https://www.anl.gov/cnm/cnm-proprietary-research).

6. User Program and Outreach Activities

Proposals are submitted via an electronic form during one of CNM's three annual open calls. The research description is captured by standard questions in one or two pages, and selections are made from CNM's various instruments and capabilities. After internal screens for safety and technical feasibility, proposals are reviewed by at least three members of the CNM Proposal Evaluation Board (PEB) for scientific merit. PEB scores and comments are ranked and allocated primarily by score until time is expended. Facility-wide, approximately 70% of submitted proposals are allocated; however, this is capability-dependent, as some instruments are in higher demand than others.

The CNM user program continually strives to attract the highest-impact users possible, including researchers from across the country and around the globe. Figure 6-1 displays the diversity of CNM users as a function of their affiliation, showing that nearly half of the approximately 600 users per year are from U.S. academia, with representation of non-Argonne users from international, industrial, and other government organizations as well. Figure 6-2 displays the diverse fields of research represented by CNM users.

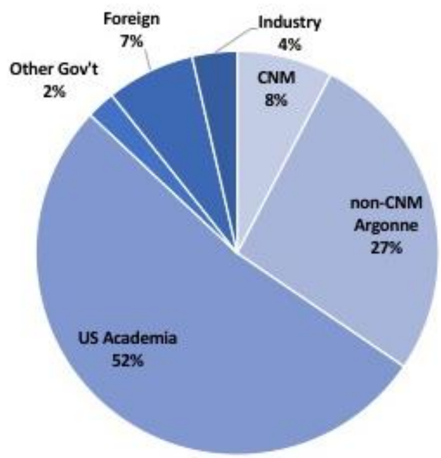


Figure 6-1: Institutional affiliations of CNM users by affiliation during FY 2020.

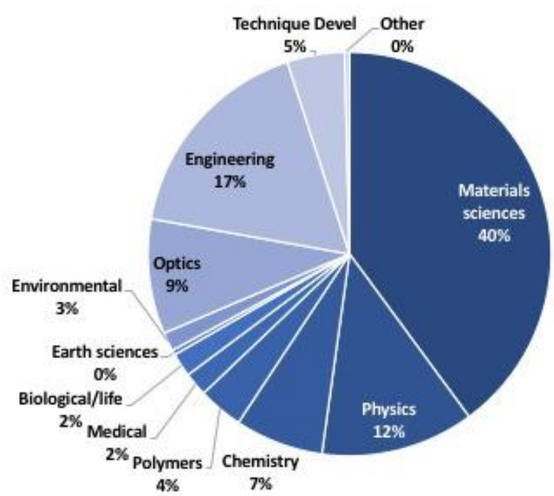


Figure 6-2: Fields of research identified by CNM users during FY 2020.

CNM continuously analyzes the suite of capabilities available to users and adds new instruments and enhancements as needed. It also removes capabilities that have become obsolete, or display little to no usage. Significant new instruments, capabilities, and enhancements acquired during FY 2016–2020 included the following (in alphabetical order):

- 4K UHV STM with Optical Access
- ADT Dicing Saw
- Dilution Refrigerator
- FEI Talos F200X TEM/STEM
- Heidelberg MLA 150 Maskless Lithography Instrument
- JEOL 8100FS Electron Beam Lithography Tool

- Low-Temperature Confocal Raman Microscope
- Magneto-electro-optical Spectrometer (MEOS)
- Magneto-optical Microscope
- Multifunctional Tribometer
- Omicron UHV 4K STM with 6T Magnetic Field
- Omicron VT-STM with Optical Access
- Photon Correlation Microscope
- Pulsed Electron Paramagnetic Resonance Spectrometer
- Rheo-XPCS at Sector 8
- Temescal FC2000 E-Beam Evaporator
- Time-resolved Spectroscopy Suite with THz Capability
- Ultrafast Electron Microscope
- Upgrades to Carbon HPC
- X-ray Synchrotron Diffraction Ptychography
- Zeiss NVision FIB-SEM

The number of refereed journal articles is one of the primary quantitative metrics of project success at CNM. The number of such journal articles authored by CNM users and staff combined in FY 2019 was more than 335, and FY 2020 is on pace for a similar number. The DOE recognizes a selection of 20 journals as conveying especially high-impact nanoscience and nanotechnology studies from the NSRCs to the public domain. In FY 2019 and FY 2020, 34% and 39%, respectively, of all CNM journal articles appeared on this NSRC high-impact journal list (final numbers for FY2020 still to be determined).

Outreach activities initiated by CNM are focused towards enhancing our existing user community and to growing the user base in areas of the highest scientific impact. An annual users meeting is held in conjunction with the APS during the second week of May to promote and enhance the latest research results within these co-located and complementary to user communities (in 2020, this meeting was changed to a virtual meeting in August due to the Covid-19 pandemic). Our latest staff science results are promoted via professional scientific meetings, invited institutional talks, press releases, our public website and social media, as well as other scientific workshops hosted throughout the year.

7. Safety and Quality

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 and that the program efficiently implements applicable ESHQ standards and requirements. The CNM staff collaborate on important ESH projects, such as the Hazardous Gas Response Team in the Nanoscience and Technology Division. 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 continues to employ a precautionary approach where there is uncertainty about the hazard potential of new chemicals, including nanomaterials. This concept guides the conduct of hazards analysis and specification of precautions when handling nanomaterials. CNM contributes to a better understanding and management of ESH concerns associated with nanomaterials and nano-enabled products.

Summary

In summary, we believe that the innovative science performed by CNM scientists shapes the user program, while at the same time, innovative user science drives future scientific directions and capability development for CNM. Sustaining this user-staff interaction, ensuring that the user base is distributed and diverse, remaining relevant to user research needs in the future, and continuing to steward and shape the direction of the nanosciences remain our most important goals going forward.