

# Center for Nanophase Materials Sciences Strategic Plan 2015–2019



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## Executive Summary

The Center for Nanophase Materials Sciences (CNMS) is a Nanoscale Science Research Center established as part of the Department of Energy (DOE) Office of Science contribution to the US government's National Nanotechnology Initiative. Located at Oak Ridge National Laboratory (ORNL), CNMS provides a diverse user community with access to state-of-the-art nanoscience research capabilities, expertise, and equipment. These resources are applied to execute a cutting-edge science program with emphasis on theory and simulation; nanofabrication; macromolecular synthesis and characterization; and understanding of structure, dynamics and functionality in nanostructured materials. The tools used include scanning probe microscopy, electron microscopies, neutron scattering, optical spectroscopy, helium ion microscopy, and atom probe tomography.

Underpinning the research activities at CNMS is the realization that there are no fundamental barriers that prevent us from reaching the most ambitious goals of energy related research, such as increasing the efficiency of photovoltaics, enhancing the energy and power densities of batteries, or more efficiently converting sunlight to fuels. However, the number of involved parameters and degrees of freedom clearly prohibit their exhaustive experimental exploration. Fortunately, computational capabilities have advanced to a point where true materials-by-design approaches can realistically be anticipated; predicting functionality of yet-to-be synthesized materials will become broadly possible. It is our belief that such approaches will first succeed for nanomaterials – i.e., at the length scale where computation, atom-precise synthesis, and imaging meet. Therefore, CNMS research aims to set the foundation that will enable researchers, including CNMS users, to predict, design and produce the (nano-)materials that are needed to address the most important energy issues.

This Strategic Plan outlines the scientific agenda that will drive the scientific progress of CNMS in the coming five years, focusing on the overall theme of *understanding and controlling the complexity of electronic, ionic, and molecular behavior at the nanoscale to enable the design of new functional nanomaterials*. A vigorous, DOE-reviewed in-house research effort is organized into three research themes and is designed to fulfill two parallel missions: to catalyze new nanoscience capabilities for energy generation, storage and use; and to create the environment needed for CNMS to act as a knowledge-driven user facility where staff expertise enables user science.

CNMS benefits from an intrinsically strong interaction with ORNL signature strengths in multiple areas and takes advantage of the distinctive capabilities of other DOE user facilities at ORNL, including the Oak Ridge Leadership Computing Facility, the Spallation Neutron Source, and the High Flux Isotope Reactor. In particular, CNMS emphasizes a strong link to *neutron sciences*, providing an environment for researchers to integrate neutron studies into nanoscience efforts. It uses its expertise in materials sciences (including polymer synthesis) and computational sciences toward the incorporation and development of the above-mentioned *materials-by-design* approaches. In order to meet these ambitious goals, it also seeks the required new advances in *imaging sciences* that build on ORNL's demonstrated leadership in scanning

probes, scanning transmission electron microscopy, He-ion microscopy, and atom-probe tomography.

Specific priorities in the studies of ultrafast phenomena at interfaces; in the fabrication strategies for 3-dimensional structures; and in monochromated, aberration-corrected scanning transmission electron microscopy are outlined in this Strategic Plan, and the corresponding equipment and staffing needs are summarized. As our strategic vision indicates, the next five years will see CNMS pursue a broad scientific agenda for energy and materials sciences in a close, dynamic collaboration with its user community. Although the in-house research is well described within the three specific research themes, these themes are expected (and designed) to evolve with time to address new opportunities, maintaining the focus of harnessing energy through nanoscience. With this focus, CNMS will continue to thrive as a critical center for advancing nanoscience throughout the scientific community in partnership with users from national laboratories, universities, and industry

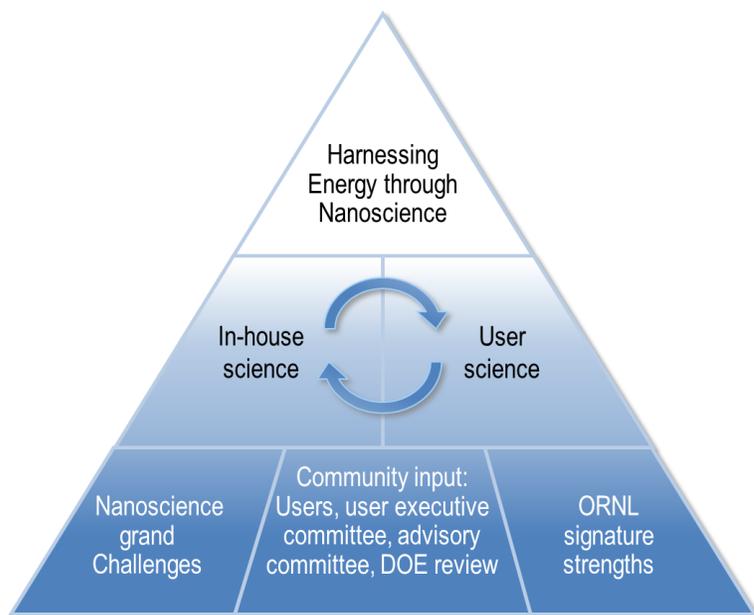
## 1. The CNMS as Research and User Facility

The Center for Nanophase Materials Sciences (CNMS) is a Nanoscale Science Research Center established as part of the Department of Energy (DOE) Office of Science contribution to the US government's National Nanotechnology Initiative and thus contributes to the goal of working toward "a future in which the ability to understand and control matter at the nanoscale leads to a revolution in technology and industry that benefits society." Co-located at Oak Ridge National Laboratory (ORNL) with the Spallation Neutron Source (SNS), the High Flux Isotope Reactor (HFIR), and the Oak Ridge Leadership Computing Facility (OLCF), CNMS benefits from ORNL's expertise in materials research and computational sciences and provides, in particular, a connection between researchers in the nanosciences and neutron sciences.

Motivating the research at CNMS is the realization that there are no fundamental barriers that prevent us from reaching the most ambitious goals of energy related research, such as increasing the efficiency of photovoltaics, enhancing the energy and power densities of batteries, or more efficiently converting sunlight to fuels. However, the number of

involved parameters and degrees of freedom clearly prohibit their exhaustive experimental exploration. Fortunately, computational capabilities have advanced to a point where true materials-by-design approaches can realistically be anticipated; predicting functionality of yet-to-be synthesized materials will become broadly possible. It is our belief that such approaches will first succeed for nanomaterials – i.e., at the length scale where computation, atom-precise synthesis, and imaging meet. Therefore, CNMS research aims to set the foundation that will enable researchers, including CNMS users, to predict, design and produce the (nano-)materials that are needed to address the most important energy issues.

Therefore, the central motivation for the work at CNMS can be summarized as a desire to harness energy through nanoscience. To this end, the CNMS mission is twofold: to enable the external scientific community to carry out high-impact nanoscience research through an open, peer-reviewed user program; and to conduct in-house research to understand and control the complexity of electronic, ionic, and molecular behavior at the nanoscale to enable the design of new functional nanomaterials (Figure 1). These two aspects of the CNMS mission are closely



**Figure 1.** With the overall goal of enabling the design of new functional materials based on nanoscale properties, the CNMS integrates in-house research and user science by building on ORNL signature strengths and taking advantage of community input.

linked and mutually benefit from each other. In particular, the partnering between key groups of users who bring outside expertise and the sustained scientific in-house effort allows the center to be a leading force in the development of new tools and methods for nanoscience, including synthesis, theory/modeling, and characterization.

Each year CNMS supports approximately 600 unique users from more than 100 different institutions spanning from academia to industry, and from around the world. The user community is diverse, ranging from students who work closely with CNMS staff—learning unique skills from experts and gaining access to cutting-edge instrumentation as they advance their research—to “partner users” who collaborate with staff to develop new capabilities and instruments that are then made available to the broad CNMS user community. About 10% of all users are theory users who work with the staff of the CNMS Nanomaterials Theory Institute (NTI) to gain access to expertise and computational resources. About 40% perform synthesis and/or nanofabrication and typically use a broad range of characterization tools to verify the quality of the synthesized materials or to investigate their novel properties. The remaining 50% of the users come to CNMS specifically for characterization, using the broad range of tools including microscopy (electron, He-ion, scanning probe), atom-probe tomography (APT), x-ray diffraction, optical spectroscopies, and other techniques.

The scope of work performed by users at CNMS ranges from the occasional routine characterization or use of an established synthesis protocol, to broader scientific questions and more complex experiments; some users access CNMS for a few days, others for several months. In the latter case, the approach chosen to solve a specific challenge often relies on the expertise of the staff researchers, who modify equipment or suggest new approaches during the user visit. Some users specifically require access to capabilities missing in their home institutions. Others push experimental or computational capabilities to the limit to obtain the most valuable results from a given approach via the in-depth interaction with expert CNMS staff and highly trained post-doctoral staff. Through such collaborative interactions, users add their expertise to that of the staff and postdocs at CNMS who serve as a resource to continuously improve the facility and its capabilities for the next generation of users.

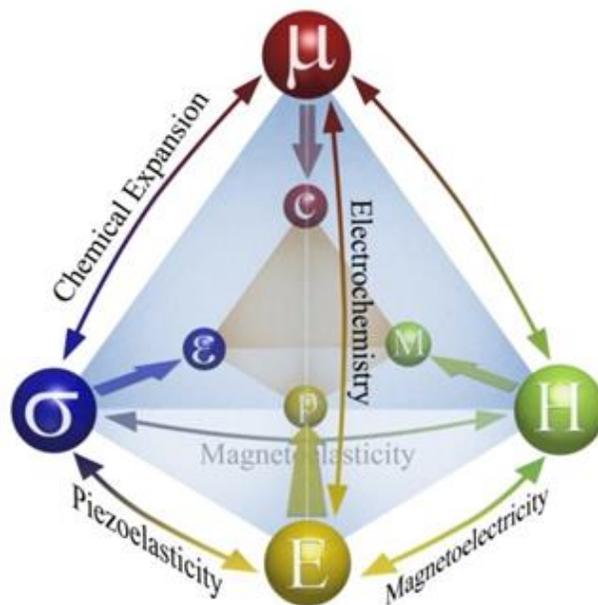
In addition to continuous informal feedback from users, CNMS receives guidance from a Scientific Advisory Committee and a User Executive Committee (UEC). The in-house research is reviewed triennially by DOE.

All researchers at CNMS are responsible both for working with users and for performing their own in-house research within the framework of the DOE-reviewed research project. Fifty percent of each staff member’s time is available for in-house research, and 20% of all equipment time is set aside for this staff research.

## 2. CNMS In-house Research

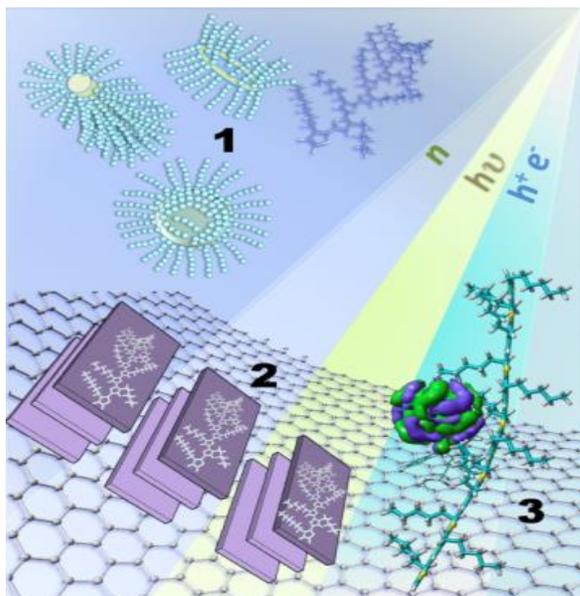
CNMS conducts in-house research to understand and control the complexity of electronic, ionic, and molecular behavior at the nanoscale to enable the design of new functional nanomaterials, with the overall goal of harnessing energy through nanoscience. The scope of this in-house research (also referred to as staff science or theme science) has evolved over the existence of CNMS and undergoes a rigorous triennial review process. Although the emphasis of this Strategic Plan is to show broad trends and strategies for addressing new opportunities, it is important to note the **three research themes** into which the in-house research effort is organized:

- The **Electronic and Ionic Functionality on the Nanoscale (EIFN)** theme *seeks to understand the link connecting the atomic-scale physics of electronic and ionic transport with chemistry and electrochemistry* (Figure 2). In this theme, electronic and ionic material functionalities are examined on the atomic scale using advanced modalities of scanning probe microscopies (SPM), and in situ/operando scanning transmission electron microscopy (STEM). The knowledge acquired is extended to the emergent behaviors at the scales of individual nanoparticles and defects and finally to the macroscale, where function can be translated into new technologies. A central thrust is to characterize and control fundamental mechanisms of coupling between electronic and ionic functionalities that underpin electrocatalysis and energy storage and conversion.
- The **Functional Polymer and Hybrid Architectures (FPHA)** theme focuses on understanding, designing, and manipulating the multiscale self-assembly of macromolecular and hybrid materials to tailor electronic transport and response. Understanding the chemical and physical mechanisms of the self-assembly of macromolecular and hybrid materials is essential for designing new materials with specifically designed functionalities. Vastly improved functionalities are required in applications that address the needs of future energy technologies, such as improved photovoltaics and battery separators. FPHA research includes the study of the role of noncovalent interactions in the self-assembly of energy-responsive macromolecular systems; investigation of the roles of interfacial interactions between organic components and substrates in directing self-assembly and the subsequent impact on optoelectronic properties; and the use of predictive theory and simulation to decipher how the chemical and physical



**Figure 2.** Ionic, electronic, elastic, and magnetic properties in functional materials are highly coupled, and the ionic link has historically received the least attention in the context of this coupling. However, ionically active materials and phenomena underpin a broad spectrum of technologies, including batteries and fuel cells.

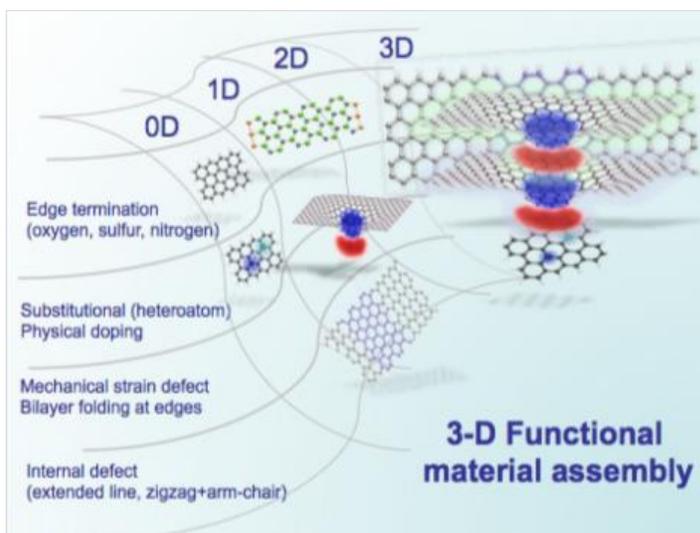
information thus encoded at the nanoscale in targeted polymer and hybrid architectures translates into structure, dynamics, and function at meso- and macro-scales (Figure 3).



**Figure 3.** The proposed research couples studies of noncovalent interaction–driven self-assembly of conjugated polymers (polythiophene shown) (1) in solution and (2) driven by well-defined (pristine) interfaces.

Tailored building blocks are synthesized and used for the experiments for comparison with (3) theory and computational simulations, which help guide and interpret the experiments. Structure and optoelectronic function are probed in situ (with neutron scattering and optical spectroscopy) and correlated with ex situ multiscale characterization, including prototype organic electronic devices.

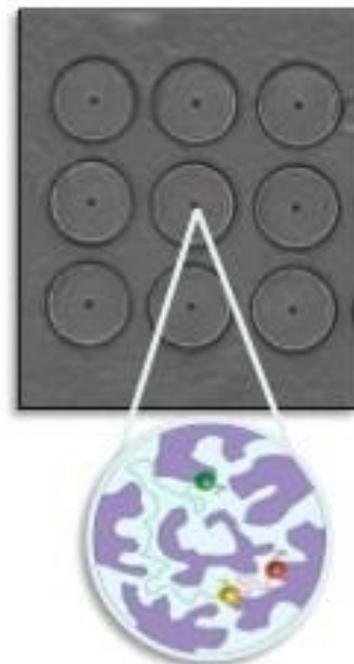
- The **Collective Phenomena in Nanophases (CPN)** theme seeks to understand and control the collective behaviors of electrons, ions, and molecules at the nanoscale to enable the design of new functional materials. In the environments of future energy systems—from dimensionally confined semiconductor materials for photovoltaics to nanoporous supercapacitor and battery electrodes—this requires understanding the behaviors that emerge when confinement and crowding force correlations between the electrons, ions, and molecules that store, transport, and release energy. This work is carried out in two specific aims: (1) understanding how atomic-scale structure, nanoscale confinement, and quantum mechanical effects impact electronic processes within nanostructures and across interfaces and (2) understanding how correlations induced or enhanced by confinement and crowding lead to collective behaviors in chemical transport and reactivity.



**Figure 4.** CPN specific aim 1: Schematic diagram illustrating the different types of edge functionalization, defect/doping types (physical, chemical and mechanical) to be examined through integrated experiment and theory for dimensionally confined materials (0, 1, 2D) and in spatially confined 3D superlattices/heterojunctions. Layered materials found in superconductors—as well as understanding of materials specificity, correlation, and confinement in these disordered electronic materials—are critical parts of the CPN research.

*Specific aim 1* focuses on the need to develop a fundamental understanding of how the properties of 2-dimensional (2D) materials and interfaces are influenced by confinement, shape, defects, and composition by using theoretical modeling and simulations in concert with experimental synthesis and characterization (Figure 4). This specific aim is differentiated from the FPHA theme by its emphasis on the building up of layers of materials to investigate how material properties are modified by out-of-plane interactions during the transition from a single 2D layer toward a 3D bulk, one layer at a time. A particularly provocative class of layered materials is those that intrinsically have strong electronic correlation, such as high-temperature superconductors.

*Specific aim 2* focuses on local correlations that are enhanced in confined and crowded chemical environments (Figure 5). Such environments are pervasive in future electrochemical energy storage systems in which electrodes with high ratios of surface area to volume or species-specific membranes are critical to achieving high energy density. The control of material architectures—such as pore and particle sizes—in the nanoscale regime is needed to control energy storage parameters such as capacity, power, charge-discharge rates, and lifetimes. However, such material architectures create environments in which crowding and confinement have numerous thermodynamic and kinetic consequences for chemical and electrochemical reaction dynamics and reactivities far removed from those found in dilute, homogenous environments.



**Figure 5.** CPN specific aim 2 builds an understanding of how correlations induced or enhanced by confinement and crowding lead to collective behaviors in chemical transport and reactivity.

## Connectivity among the Three Research Themes

CNMS is competitively positioned to engage in frontier nanoscience research and development, and it does so by fostering the links between the three themes outlined. Thus it aims to vigorously develop its cross-cutting scientific approaches by capitalizing on new synergies and pursuing emerging areas of nanoscience. For example, the general emphasis on *energy storage and conversion* spans across all three themes—investigating the link between electronic and ionic motion in the EIFN theme; synthesis and understanding of energy-responsive materials, including polymer electrolytes and organic electrodes, in the FPHA theme; and studies of dimensional and spatial confinement in CPN, with important work on supercapacitors. In the FPHA theme, one focus will be on understanding synergistic (or collective) behaviors of polymers in different settings, including confinement and the application of external stimuli (fields, forces, temperature, illumination), to harness properties for important energy-related applications. Another will be investigating the role of interfacial interactions between organic components and substrates in directing self-assembly and the subsequent impact on optoelectronic properties. In the CPN theme, new scientific activities will revolve around

concepts for accelerated materials discovery in 2D and layered materials. Such materials are an ideal materials-by-design platform that ties together theory, functionality, and synthesis through elegant characterization techniques. An emerging area of interest at CNMS is the convergence of synthesis with in situ real-time diagnostics, characterization, and theory to address the need for rapid synthesis and characterization of 2D nanosheets and their functional inorganic/organic hybrids. The properties of 2D layered materials vary dramatically as the nanosheet layer number becomes small, with remarkable electronic, magnetic, and optical properties emerging. However, mastering the synthesis and properties of these materials requires a detailed understanding of their interactions with substrates—providing the bridge to the interfacial studies in the FPHA theme. Capabilities within CNMS allow the synergistic convergence of theory, characterization, and synthesis necessary for breakthroughs in the synthesis and property assessment of 2D materials. The discovery of new functional 2D materials has amplified significance: such well-characterized surfaces can then also be exploited as epitaxial substrates for the assembly of custom-synthesized molecular and macromolecular hybrid thin films with novel or enhanced properties for multiple applications such as organic electronics, catalysis, or sensing.

### **3. Integration into ORNL Missions: Neutron Sciences, Materials by Design, Imaging**

Neutron sciences, materials-by-design strategies, and novel approaches in imaging are all focus areas of ORNL. The work of CNMS, both its in-house research and its interactions with the user community, directly contributes to and benefits from these areas of emphasis, as described in the following sections.

#### **The Link to Neutron Sciences**

The direct proximity of CNMS to ORNL's two neutron sources, HFIR and SNS, provides a unique opportunity to use neutrons as probes to answer nanoscience questions. In fact, 18% of all CNMS users are also users of either SNS or HFIR or both. We are actively taking steps to increase the interactions between the neutron and nanoscience efforts, in both CNMS staff science and user projects. For example, ORNL has established a Soft Matter Council of members from both the nanoscience and neutron science areas within ORNL that has the mandate to identify areas of common interest and opportunities. In addition, simple administrative steps have been implemented, such as a simplified access route for CNMS users to SNS and HFIR and vice versa (discussed in Section 4). Neutron–nano interactions are currently strongest in the area of soft matter research, in which CNMS deuteration capabilities are a key resource for the neutron scattering programs, and the sensitivity of neutrons to light elements allows the investigation of assembly, structure, and dynamics in complex macromolecular systems. The demand for the selective deuteration capabilities will continue to increase as the number of soft-matter users at both facilities increases. In parallel, CNMS is investigating the impact of deuterium substitution on functional properties, e.g., via electron-phonon coupling.

CNMS is partnering with SNS/HFIR to develop new capabilities for neutron studies of materials, including specialized *sample environments* and new characterization techniques that can be used in concert with neutrons to provide multi-dimensional information on material structure and function. Similarly, CNMS provides a key component to future neutron studies of soft matter and bio-inspired materials via the fabrication of *nanostructured templates* having lateral dimensions sufficient for neutron experiments. As more instruments become integrated into the neutron user program, and as plans are made for a second target station at SNS, the interactions between CNMS and the Neutron Sciences Directorate are growing.

As an illustrative example, neutron reflectometry is used in critical experiments to provide depth information for layered materials. This is particularly the case in the study of assembly and self-organization of macromolecular and polymeric materials (where the specialized sample environments provide simultaneous optical and spectroscopic information), or in investigating electronic and magnetic reconstruction at atomically abrupt interfaces within an oxide heterostructure. Complementary techniques, such as scanning-probe-based 3D force imaging to study ionic layering in liquids, or real-space cross-sectional transmission electron microscopy (TEM) for epitaxial structures, will benefit from (and contribute to) these neutron capabilities.

CNMS research in energy storage and conversion is another specific example of the benefits of proximity to the ORNL neutron sources. Issues of ionic transport in inorganic solids, including lithium ions and protons, are investigated using the SNS instruments NOMAD instrument (Nanoscale-Ordered Materials Diffractometer) and POWGEN (powder diffractometer) for structure resolution. Dynamic ionic transport studies within the EIF theme and in user work take advantage of quasi-elastic scattering on the SNS BASIS (Backscattering Spectrometer). Additionally the SNS VULCAN (Engineering Materials Diffractometer) instrument has provided the capability for operando charge and discharge studies of whole battery cells to understand structure evolution within a cell, and an in situ high-temperature environment for real-time characterization of structure and property evolution for energy-related materials.

The recently commissioned SNS VISION vibrational neutron spectrometer provides an opportunity for the study of in situ catalysis and study of active sites in materials difficult to probe using other spectroscopic techniques. CNMS scientists are in a unique position to help SNS staff develop environmental capabilities that will attract users studying catalytic and energy-related processes to both facilities. CNMS provides unparalleled local capabilities for materials synthesis, and CNMS researchers work closely with SNS scientists to develop capabilities of interest to users of both facilities.

Closely related to the interactions with the neutron community, and taking advantage of the sensitivity of neutrons to spins, is our effort at CNMS to strengthen and broaden research on *magnetism and magnetic materials*. On the synthesis side, laser deposition of oxide layers and molecular-beam epitaxy of metallic materials strategically position us to take advantage of CNMS characterization strengths in measuring magnetism and magneto-transport and in scanning electron microscopy with polarization analysis (SEMPA). New methods in spin-polarized scanning tunneling spectroscopy and cutting-edge approaches to extracting magnetic

information from electron energy loss spectroscopy (EELS) data (discussed later) will play a significant role in connecting neutron results with spatially resolved information. CNMS is leading the development of these approaches, making them accessible to a broad range of users. Theoretical contributions, including work on multiple orbital models of transition metal oxides with realistic interactions, help researchers understand and develop experiments by studying not only static properties at zero temperature but also dynamical properties at finite temperature.

## **Materials by Design**

As the ability to computationally predict and design specific functionality advances at CNMS, the ability of its users to discover revolutionary new materials will be expedited. The NTI at CNMS will lead the development of new computational methods of examining systems with ever increasing complexity, taking advantage of petascale (and eventually exascale) computing capabilities available at ORNL. NTI staff are actively involved in both theoretical and computational algorithmic developments to facilitate and enable advanced molecular simulations that efficiently exploit ORNL's world-leading high performance computing facilities.

Materials-by-design approaches not only rely on theoretical/computational guidance but also necessitate a fundamental understanding of synthesis methods and multi-scale visualization of physical properties. The importance of imaging is described in the next subsection. For synthesis, in situ diagnostics play a key role; and CNMS will maintain and solidify its strength in precision synthesis, including that of molecular building blocks, polymers, and co-polymer architectures, as well as epitaxial heterostructures. CNMS has established broad expertise in synthesis of macromolecular and hybrid systems and specialized nanomaterials, ranging from nanoparticles to 2D and 3D materials. In the future, we will expand our synthetic skills—such as using flow chemistry and the incorporation of heteroatoms (e.g., fluorine, boron) to understand the basis of directed-assembly and self-assembly of materials into designed architectures—to enhance ionic and electronic transport, which is central to the development of new materials for future energy technologies. In addition, CNMS strengths in nanofabrication will enable new capabilities—essentially new “control knobs”—for understanding and tuning selectivity and reactivity. The area of interfacial nano-chemistry is tied to the theory-guided design of compatible substrate–molecule and molecule–molecule interactions to drive self-assembly and polymerization, leading to new materials and properties.

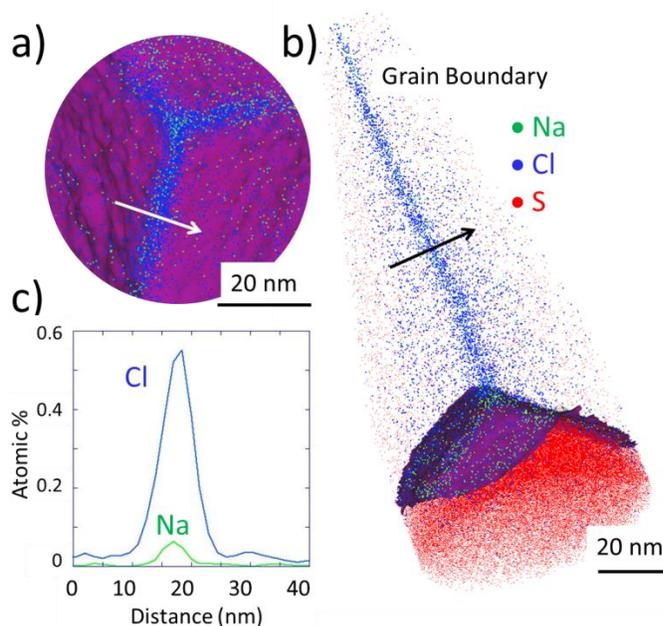
Software (code) developments are often key to materials-by-design approaches, but they are typically beyond the scope and mission of CNMS. However, the NTI links directly to researchers funded by other agencies, in particular DOE's Advanced Scientific Computing Research program, and thus lends CNMS a voice in the future development of codes without directly performing this work.

## **Imaging**

A broad range of imaging approaches is needed for success in nanoscience, both the staff science pursued in the scientific themes and the science carried out by the user community. Integrating the advanced microscopy capabilities that were previously part of the Shared Research

Equipment (ShaRE) user program, CNMS now combines key strengths in SPM, TEM, STEM, SEMPA, He-ion microscopy (HIM), and APT. Within SPM, low-temperature and variable-temperature scanning tunneling microscopes (STMs) are designed and built fully in-house. Based on our expertise in four-probe STM, a scanning tunneling potentiometry method has been developed, which is now being extended to spin-polarized probes. Similarly, band excitation and multidimensional spectroscopic modes for probing bias- and temperature-induced phase transformations and electrochemical processes have created new opportunities for exploration in areas as diversified as ferroelectrics, multiferroics, and energy storage/conversion. These capabilities have propelled CNMS to the forefronts of these fields and engendered a vibrant user program.

Across many of these imaging platforms, materials are not simply imaged in the sense of determining atom locations but rather are interrogated to reveal spatially resolved maps of physical properties and functionalities (see Figure 6). Local stimuli (e.g., electric fields, strains, electron beams) can reversibly probe a material's response or produce localized modifications, chemical reactions, or nanostructure assembly. Mapping of physical properties results in multi-dimensional data sets for which the historically successful analysis approaches of fitting and parameter extraction have become inadequate, especially in cases where a phenomenological parameterization at all locations in a sample cannot be performed without loss of information. This points to the need for “deep data” approaches, an area in which the close link between theory, computation, and imaging positions CNMS well to provide the required breakthroughs.



**Figure 6.** A 3D APT reconstruction shown from the top (a) and side (b) of a triple CdTe grain boundary (GB) meeting the CdS/CdTe interface within a CdTe solar cell device. Each colored sphere in the APT map indicates the position and type of atom detected (only Na, Cl, and S atoms are displayed for clarity). An 18% sulfur isoconcentration surface (displayed as a magenta surface) was drawn to separate the CdTe and CdS layers. The images clearly show Cl segregation within the CdTe GBs, and Na segregation at the CdS/CdTe interface. A 1D concentration profile (c) across a CdTe GB reveals that Na segregation of  $<0.1$  at. % can be detected by this technique. Na segregation at the CdS/CdTe interface and within CdTe or CdS GBs is below the detection limit of analytical STEM and therefore has never been detected using those techniques.

The CNMS vision to provide staff scientists and users with forefront tools and approaches is supported by our plans to

- continue to develop and implement state-of-the-art techniques for probing phonons and optical excitations, magnetic and electrical responses, and lattice vibrations through the acquisition of an advanced monochromated aberration-corrected STEM (MAC-STEM) as described in Section 4
- advance the scientific basis of HIM and implement mass spectrometry approaches into HIM so as to provide spatially resolved and surface-sensitive chemical information
- emphasize continued improvements for in situ and operando functional imaging and spectroscopy of materials processes at high spatial and temporal resolution
- enhance CNMS leadership capabilities in APT by emphasizing nanomaterial studies on the next-generation atom probe with significantly enhanced collection efficiency (from 37% to 80%)

Linking many of these approaches are efforts to combine data streams (e.g., APT data with STEM chemical and lattice imaging and spectroscopy data) to provide unprecedented 3D, multi-modal insights into nanomaterials structure and behavior.

The recent establishment of ORNL’s Institute for Functional Imaging of Materials (IFIM), to which CNMS is a key contributor, ensures that CNMS imaging science works in concert with other imaging efforts across ORNL (including particularly chemical imaging and STEM) and data analytics capabilities. Therefore, the IFIM provides a platform for enhanced information exchange, efficient resource utilization, and identification of common needs across the various imaging platforms.

## **4. Strategic Enhancements of the In-house and User Research Environment**

### **Maintaining a Vibrant User Environment**

CNMS user satisfaction, as measured through its annual user satisfaction survey, has been very high and is still steadily improving: in the most recent survey (FY 2013), approximately 40% of the users took time to respond, and more than 95% of the responses to all questions on the survey were “Satisfied” or “Very Satisfied.” CNMS will strive for further improvement by actively soliciting user feedback and taking action to respond to improvement opportunities identified by the user community. CNMS benefits from a very engaged UEC that is elected by the users and convenes monthly conference calls to discuss topics and identify issues affecting the user experience. Recent actions taken directly as a result of UEC recommendations include implementation of an online Suggestion Box and a “Thank a Staff Member” page to collect spontaneous user input and stimulate UEC recommendations to CNMS management. The UEC is now responsible for planning the annual user meeting, including identifying topics, inviting speakers, and selecting abstracts. CNMS leadership will continue to pursue extensive engagement with the UEC as a key component of the strategy to enhance the user experience. Other primary venues that the UEC and CNMS management plan to use to gather and interpret feedback on user needs and expectations are the annual user meeting itself, particularly panel

discussions and staff presentations; and topical workshops on strategic areas for research growth and capital investment, some of which are cited in the section “Specific Priorities” below.

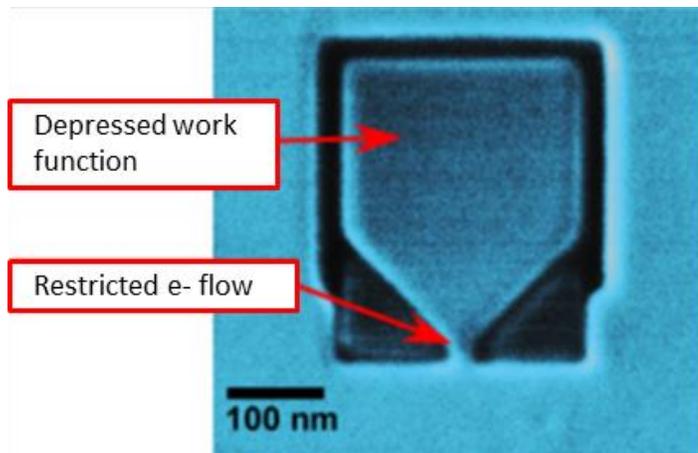
CNMS also continues to improve its outreach to neutron scattering users and develop greater visibility within that growing community. For several years, CNMS has offered its users an opportunity to request neutron scattering time as part of a CNMS user proposal; more recently, an equivalent mechanism has been implemented to provide streamlined CNMS access to the neutron user community as part of the neutron proposals. CNMS thus continues to support neutron scattering user projects either through its Rapid Access proposal process or as regular proposals, in both cases accepting the peer reviews of the neutron scattering proposal.

In the coming five years, CNMS will continue to vigorously develop science-led capabilities that will ensure it remains a powerfully enabling resource for the user community. The *close integration of synthesis, imaging/characterization, and theory/modeling/simulation* that characterizes CNMS staff research in the three scientific themes leads to a comprehensive environment in which users can simultaneously take advantage of a multitude of capabilities. CNMS will continue to solicit user input as described to inform decisions on developing new research directions and strategic capital investments that will strengthen the user research portfolio. It will use feedback from the Scientific Advisory Committee, the UEC, and the DOE triennial review process. Metrics such as number of users for each research area, and number of user publications resulting from such projects, are tracked and used in the decision making process.

Building on scientific breakthroughs in *electrical energy storage* at CNMS, new capabilities in electrochemistry and battery research will be made available to researchers. Nanomaterials synthesis capabilities will be provided to the user community for air-sensitive energy nanomaterials. A new laboratory has been established that consolidates materials synthesis and electrochemical characterization for energy storage. Building a link between traditional heterogeneous catalysis and electrochemistry will meet the blossoming catalysis research needs for energy storage and conversion. *In situ characterization* tools as described in the context of imaging will continuously evolve to provide users with unparalleled resources. Other characterization methods, such as confocal and near-field optical spectroscopy, will be developed as cross-platform *real-time* probes. They will not only reveal the local properties of materials after synthesis but also clarify their properties during growth and assembly and how they respond functionally upon exposure to environmental effects during simultaneous characterization in situ within neutron beams or scanning probes. To this end, CNMS is continually developing new capabilities, such as an ultrafast white-light pump-probe microscope to study both interband and intraband exciton dynamics at tailored interfaces, and multimodal optical/electronic spectroscopy across multiple length/time scales.

As mentioned earlier, significant enhancements are envisioned in the area of imaging, with new instrumentation and scientific advances needed in electron microscopy (MAC-STEM), the addition of mass spectrometry approaches into HIM, continued improvements for in situ and operando functional imaging and spectroscopy, and increased collection efficiency in APT.

While these refer to future equipment and investments, the current capabilities in HIM and APT are just now becoming fully recognized by the user community. For HIM, recent unpublished work demonstrates its unparalleled capabilities in imaging of soft matter and patterning of ultra-small features without the need for a resist layer or etching, thus exceeding the possibilities of e-beam lithography (Figure 7). APT is being made available to the broader CNMS user community as a result of recent efforts to more fully integrate the technique in nanoscience research and of enhanced staffing.



**Figure 7.** Diode structure obtained by  $\text{He}^+$  milling in CVD-grown single-layer graphene on  $\text{SiO}_2$

Equally significant is the development of new *synthesis capabilities and synthesis expertise*. An area of particular importance for CNMS in-house research, as well as for CNMS and neutron users, is well-defined (including branched) polymers, selective deuteration, and nanocarbon structures. As research priorities evolve, a new emphasis will be placed on novel 2D materials (“beyond graphene”), including 5D transition metal dichalcogenides (TMDs), assembly of 2D materials into complex structures using Van der Waals epitaxy, and a future emphasis on plasmonic and photonic phenomena at the nanoscale. Emphases in nanofabrication will include the creation of innovative platforms to investigate nanochemistry and to provide the neutron community with the required structures (necessitating large-scale lateral registry of nanoscale patterns). The particular focus on 3D approaches is discussed later.

With the recent (FY 2014) addition of a Quantum Design Physical Properties Measurement System to the already available superconducting quantum interference device (SQUID) magnetometer, CNMS will be able to provide users with a more complete suite of instrumentation for electromagnetic and electro-optical measurements, including magnetism and magneto-transport. Such capabilities are of particular value to those researchers who also use neutrons as probes of magnetism.

Computational efforts that develop efficient mathematical algorithms and advanced computing techniques to optimize core simulation codes on the massive computing platforms at ORNL’s National Center for Computational Sciences will continue to advance our ability to perform realistic, accurate first-principles nanomaterial simulations (for soft matter, strongly correlated materials, and electronic structure calculations), directly integrating computation with experiment in support of user science.

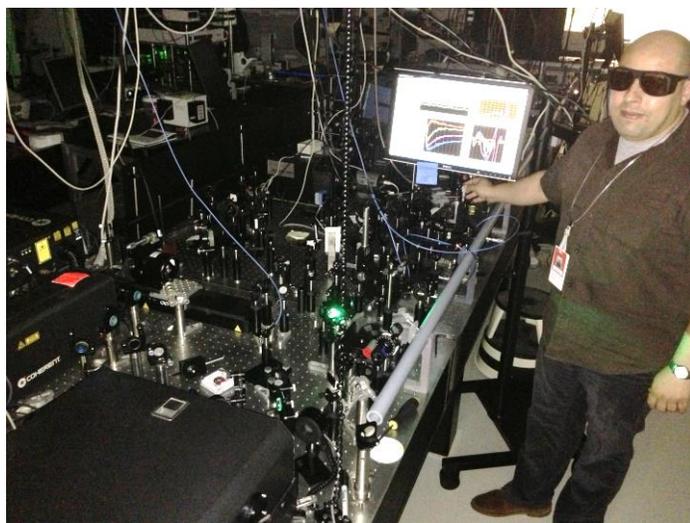
## Specific Priorities

Three specific priorities encompass a broad range of priorities dictated by new directions in user research, as well as those required for multiple aspects of the three research themes of CNMS in-house science.

### 1. Studies of ultrafast phenomena at interfaces

Fundamental understanding of *energy flow at interfaces* is central to nearly all next-generation energy conversion and utilization technologies. Understanding energy transport across atomically thin interfaces requires combined capabilities to measure and simulate the same *ultrafast dynamical events* both experimentally and computationally. Two-dimensional nanosheets of TMDs offer exquisitely well-described model interfaces for this purpose. They are semi-transparent, making them amenable to both optical and electron spectroscopies, and they are tractable in ab initio computational simulations using a reasonable number of atoms. Moreover, the spatial confinement of these 2D systems, realistically a few atomic layers, results in several intriguing optical properties: a transition from indirect to direct bandgap, formation of strongly bound excitons and charged excitons, coherent electronic coupling, and coupled spin-valley band structure. Two-dimensional layered materials that are synthesized and exquisitely characterized at CNMS afford a unique opportunity to address the major scientific challenges governing ultrafast energy flow dynamics at interfaces that are crucial to optoelectronic applications such as solar photovoltaics.

The fundamental understanding of optical interactions of laser radiation with materials is central to our ability to probe their electronic and vibronic energy levels and relaxation pathways, and ultimately to control the energy flow at interfaces. CNMS is currently developing microscope-based approaches for transient pump-probe absorption and reflection spectroscopy using 40 fs pulses of tunable laser light and photogenerated white light continuum (Figure 8). To understand



**Figure 8.** CNMS postdoc Aziz Boulesbaa and 40 fs pump-probe spectroscopy setup.

the ultrafast photogeneration and separation of carriers at interfaces crucial to optoelectronic applications, two microscopes will probe both interband (vis-ultraviolet) and intraband (infrared) absorption of light to reveal the generation and dynamics of excitons within micrometer spatial regions in 2D crystalline nanosheets, polymers, quantum dots, and their heterostructures. To understand the mutual interactions between layers or nanostructures within heterostructures that govern ultrafast carrier dynamics, complementary studies using the high-resolution tunable Raman

spectroscopy setup at CNMS will characterize the very low-frequency ( $<50\text{ cm}^{-1}$ ) vibrational modes that reveal the Van der Waals and charge transfer interactions for direct comparison with advanced ab initio calculations.

In addition to revealing energy flow across material interfaces, the extremely high laser intensities available by focusing femtosecond laser pulses to micron spot sizes will be explored to induce defects, modify and dope materials, and pattern materials by both thermal and photolytic processes. Combining these studies with the parallel development of ultrafast spectroscopy techniques (e.g., Raman spectroscopy, second-harmonic generation, and sum-frequency generation) to probe material structures and electron dynamics affords the possibility of in situ control of these laser modification processes. Of special interest are polymers that are optically transparent in the linear regime, but in which multiphoton absorption with two overlapped beams can be used to initiate and terminate polymerization reactions with resolutions beyond the diffraction limit. These principles are central to (commercially available) 3D-printing tools that can create arbitrary structures and patterns central to CNMS core research in all three research themes (see item 2 below). Building on FPHA theme research, plans are to take advantage of the capability to synthesize photoactive polymer and small molecule building blocks to explore the laser direct-write materials design and fabrication of conducting polymer and hybrid polymer/inorganic structures; this will enable the exploration of novel optoelectronic, chemical, and biological functionalities in 1D, 2D, and 3D.

## **2. Fabrication strategies for 3D structures**

The identification of “fabrication strategies for 3D structures” as a key opportunity is a particularly clear example of how interactions between in-house research and user efforts lead to the formulation of strategic needs. In fact, specific aim 2 of the CPN theme focuses on building an understanding of how correlations induced or enhanced by confinement and crowding lead to collective behaviors in chemical transport and reactivity. This research goal is pursued by leveraging nanofabrication to create controlled architectures in which transport and reactivity may be characterized in a wide array of crowded/confined environments. To address this topic with the user community, CNMS held a workshop (May 2013, attended by 49 researchers representing 9 different institutions). A key outcome from this meeting was identifying the need for finer control in all three spatial dimensions (beyond the capabilities of CNMS and other facilities in 2+ dimensions, i.e., fine control in the x, y dimensions but less flexibility in z). The multiscale surface textures enabled by such control will play an increasingly important role in studies of fundamental mechanisms controlling multiphase flows, imbibition, dewetting, mass transport, and chemical separations. In particular, anisotropic surface textures based on deterministic arrays of chiral, tilted, and low-symmetry features offer unique opportunities in studying very intriguing effects of geometrical bias on various surface and interfacial phenomena, including ratcheting effects, multiphase flow rectification, asymmetric friction, and directional dewetting. The challenge of creating arbitrary complex 3D structures can be addressed much more broadly and efficiently with the advent of novel 3D micro- and nanofabrication strategies that use 2-photon polymerization.

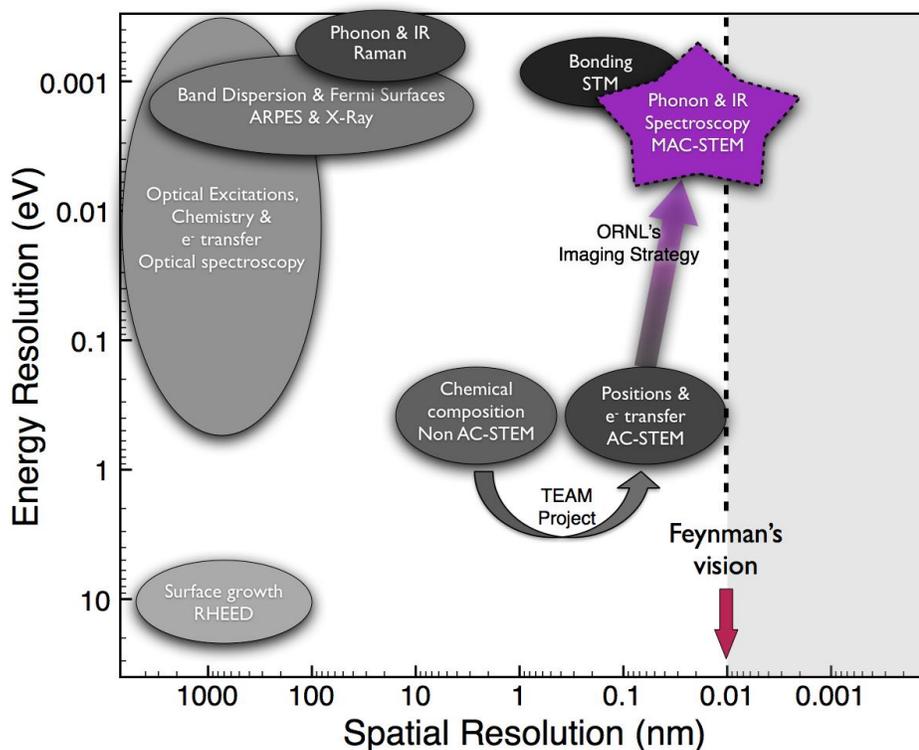
Porous, high-surface-area structures can be created in ultraviolet-curable polymers optimized for structure formation. These can be converted to SiO<sub>2</sub> and silicon elements using single and double inversion techniques that capitalize on existing atomic-laser deposition, reactive ion etching, and deposition capabilities within the nanofabrication research lab. Subsequent chemical modification of surfaces will facilitate the attachment of functional polymers, synthesized at CNMS, to the scaffold surface. Furthermore, chemically modified porous materials with deterministic 3D structures can be used to study the effects of synthetic crowding and confinement on chemical reaction systems. Integration with conventionally machined fluidic architectures will add an additional refinement in the control of porosity within open fluidic systems and facilitate the transport between confined fluidic compartments.

High-resolution 3D structures may also be fabricated via electron beam–induced deposition (EBID), in which a volatile organometallic precursor decomposes in a controlled manner under electron impingement, thereby depositing materials in the area local to the well-defined electron probe. A closely related technique using He<sup>+</sup> (which has the potential of achieving a purer product and a more efficient conversion of the precursor into the desired material) has been demonstrated, and CNMS HIM is now being modified to provide this capability. CNMS has pursued complementary electron techniques using the dual-beam focused ion beam already available in the CNMS nanofabrication research laboratory. These two world-class instruments will provide EBID and ion-milling capability to users that are unavailable anywhere else.

### **3. Monochromated, aberration-corrected STEM**

Electron microscopy, and more specifically STEM, continues to play a key role in the understanding of materials, enabling researchers to accurately determine the positions of atoms within a solid and even to simultaneously determine their chemical identity and bonding configuration using EELS. Therefore, CNMS microscopy tools are among the most heavily subscribed and most productive pieces of equipment at the center. Microscopy techniques have fundamentally changed how we can interrogate complex materials at the atomic scale, and the next advances in this field promise even further-reaching breakthroughs. In fact, the improvements in energy resolution and analysis of EELS are approaching the point where it will be possible to probe phonons and optical excitations, and even the magnetic characteristics of materials at the atomic scale; and the spatial resolution of STEM imaging will soon allow observation of lattice vibrations in real space (Figure 9). This will make it possible, for example, to accurately determine the paths of heat flow nanostructures and measure the degree of phonon scattering at single interfaces and defects. Spectroscopic measurements combined with high spatial and energy resolution will make it possible to determine bandgaps, as well as optical and magnetic properties near defects and interfaces and in complex nanostructured materials, such as those becoming increasingly important in solid-state lighting, solar cells, fuel cells, and battery applications.

Theoretical predictions for 5th-order aberration correctors indicate the possibility of larger convergence semi-angles (as high as 50 mrad) and a corresponding increase in spatial resolution from the current ~0.6 Å to ~0.3 Å, so that atomic positions within a material could be measured



**Figure 9.** Physical information obtained by different spectroscopy techniques at different energy and spatial resolutions. The next generation of MAC-STEM will be able to reveal phonons and optical excitations of materials at the atomic scale simultaneously with their structures, chemistries, and bonding configurations.

with much higher precision than the current 0.1 Å. This would allow not only real-space observations of lattice vibrations but also the measurement of chemical expansion strains, ferroelectric distortions, and bond lengths and bond angles in solids.

At the same time, advances in EELS will soon make it possible to perform spectroscopic investigations of a material's properties not only in spatially averaged measurements (particularly including synchrotron x-ray spectroscopies) but also in an atomically resolved approach using STEM. Our strategic vision is to push the limits of EELS in the electron microscope toward single-digit milli-eV (meV) energy resolution while maintaining an atomic-size electron probe, to ultimately reveal the link between atomic structure, bonding, local optical and plasmonic response, phonons, magnetism, and vibrational states of materials, all at the atomic scale. Achieving an EELS energy resolution below 10 meV in the electron microscope would enable the study of localized phonons and molecular vibrations having energies as low as 20 meV. Likewise, energy gaps, as well as the optical (and magneto-optical) properties of a material, could be studied in real space at an unprecedented energy range with improved energy resolution, combined with an unmatched spatial resolution.

It is important to note that enhancing the energy resolution in EELS with a monochromator immediately results in minimizing the chromatic aberration,  $C_c$ , which is the limiting aberration at low acceleration voltages. Therefore, our approach will prove particularly advantageous as we

continue to push electron microscopy into a lower regime of acceleration voltages (i.e., 20, 30, or 40 kV) while maintaining an atomic-size probe. The motivation for low-voltage microscopy is, of course, reducing damage to the specimens, particularly for studying defects in 2D materials, organic materials, and polymers. For instance, organic molecules could be supported on graphene (or another 2D material); and their electronic and optical properties, as well as molecular vibrations, could be revealed at the atomic scale. Similarly, investigations of few-atom clusters deposited on a 2D material would have huge implications for understanding mechanisms of catalysis related to cluster morphology, environment, and stability.

Recent advances in electron microscopy have demonstrated that EELS is also sensitive to magnetic quantities, such as spin and orbital moments, through the study of the EELS near-edge fine structure. Recently, it was also shown that by using a patterned objective aperture, sub-nanometer vortex beams (electron beams carrying orbital angular momentum) can be created. With these discoveries, it will become possible to probe the magnetic properties of materials with unprecedented spatial resolution.

## 5. Instrumentation and Space Utilization

The previous sections, especially the description of strategic enhancements to the user and in-house research environment, clearly indicate a need for continued investments in future instrumentation. This includes in particular *major investments in electron microscopy and APT*. Additional investments are needed to succeed in the goals described above, particularly

- Nanoscribe's Photonic Professional 3D Laser Lithography system
- instrumentation for ultrafast spectroscopy
- environments for in situ and *operando* electron microscopy
- mass spectrometry upgrades to HIM
- sample environments and associated characterization tools for experimentation on neutron beam lines

Additional and significant investments are needed to maintain the existing suite of instrumentation and continuously replace equipment when maintenance becomes impossible or the instruments become obsolete, to provide users at a minimum with current-generation capabilities. These include the purchase of computing resources (managed through the Oak Ridge Institutional Cluster), the numerous highly used pieces of equipment for characterization and fabrication, and routine laboratory equipment.

With the cost of liquid helium and the reliability of supply being significant issues, the purchase of helium recovery units is being considered. In particular, a free-standing unit to supply, for example, the SQUID magnetometer has been evaluated as an alternative to a more expensive building installation that would recover helium from all instruments, including the nuclear magnetic resonance instrument. Recovering helium has become much easier because modern re-

liquefiers require very little maintenance and staff attention (unlike when CNMS first began operation).

Given the high cost of maintaining certain types of equipment (i.e., the maintenance contracts), CNMS has transitioned some of the more conventional and routine instruments that were formerly part of the ShaRE user facility to a “service center” mode of operation. Under this arrangement, access to such instruments is via cost-recovery rather than through peer-reviewed user proposals. Exceptions are made for certain capabilities required by users. This arrangement applies exclusively to equipment for which there has been limited demand from the user community or to previous ShaRE capabilities that overlap with existing CNMS resources:

- FEI-Philips CM200 TEM/STEM (19 years old).
- FEI Tecnai 20 TEM (11 years old).
- JEOL 6500 FEG-SEM (10 years old). There is a special provision to guarantee access to CNMS users requesting electron backscatter diffraction and energy dispersive x-ray spectroscopy capabilities.
- S4800 FEG-SEM (9 years old). There is a special provision to guarantee access to CNMS users requesting electron beam induced current capabilities.

Space at CNMS is somewhat limited by the boundaries of the building, which puts a particular strain on activities that require ground floor low-noise/low-vibration environments. CNMS has begun locating some of these instruments in ORNL’s Advanced Microscopy Laboratory on the main ORNL campus, paying for that space through the regular space charge cost model. However, given the increased sensitivity and performance of many of our key characterization tools, a future expansion into low-noise/low-vibration space (i.e., new construction) will become necessary to provide users state-of-the-art research opportunities. In other cases, the space issue is being addressed through the natural evolution of research in which one subject gains in importance at the expense of another. A specific example in this context is the establishment of the battery processing and testing laboratory, which is being set up in space formerly used primarily for the solvothermal synthesis of nanomaterials, an area in which user demand has decreased.

## **6. Staffing Plans**

Meeting CNMS goals requires that the facility employ outstanding scientists, engineers, and support/operations staff. Researchers hired into CNMS become part of a highly collaborative and productive research environment with outstanding facilities and the opportunity to focus on important research areas. They also interact directly with leading research groups through the CNMS user program and are encouraged to participate in major national and international conferences. It is therefore not surprising that staff members from CNMS at all levels have been recruited for opportunities outside ORNL and that CNMS is therefore constantly re-hiring and

thus bringing individuals with diverse backgrounds into our organization. At the same time, CNMS strives to assist with the career development of research staff into new or expanding areas of nanoscience that directly impact our mission and have high potential to engage an expanding user community. Part of the future success of CNMS will be linked to expanding opportunities for outstanding researchers within the program. CNMS also strongly encourages its researchers to take advantage of Laboratory Directed Research and Development (LDRD) opportunities to develop their own ideas if they are aligned with the mission of the CNMS but outside the scope of the peer-reviewed theme science. Such venues encourage creativity and contribute to staff retention and at the same time provide a testing ground for novel ideas that may eventually be rolled up into the user program or the theme science if they prove successful. Current LDRD and seed-project examples include spin-polarized scanning tunneling potentiometry, “deep data” approaches for microscopy data, and nanostructured templates for neutron research on membrane structures.

Since its inception, CNMS has pursued a vision to build a leading polymer science group based on its unique combination of capabilities in precision synthesis and deuteration, neutron scattering, and macromolecular modeling/simulation. In active recognition that this vision continues to be central to the CNMS agenda, CNMS is recruiting two outstanding macromolecular scientists to further establish and strengthen the research in this area. In particular, we seek to expand the integration between chemical synthesis, polymer physics, and neutron scattering sciences. A Soft Matter Council reporting to ORNL’s Deputy Director for Science has been established not only to assist in that search but also to help develop future research directions, recognizing the direct link between staffing decisions and research strategies.

Strategic hiring funds, available through ORNL’s LDRD program, are particularly attractive when the aim is to hire junior researchers to work in parallel with senior staff to ensure transfer of knowledge and expertise. CNMS has taken advantage of the opportunity to hire a junior staff member in APT. Similarly, CNMS actively pursues opportunities within ORNL’s named fellowship programs, particularly the Wigner and Lianne B. Russell Fellowships (which bring in recent doctoral degree recipients of exceptional ability to pursue research programs within their areas of interest and expertise) and the Weinberg Fellowship (for early career scientists and engineers with interests in energy and energy-related science and technology challenges).

## 7. Outlook and Future Opportunities

As described in this document, we have developed the strategies that are needed for the CNMS to set the foundation that will enable researchers, including CNMS users, to predict, design, and produce the (nano-)materials that are needed to address the most important energy issues. Therefore, our work will contribute to true materials-by-design approaches, i.e. leading to the prediction of functionality of yet-to-be synthesized materials. Such approaches will become

feasible first at the nanoscale, i.e., precisely where our capabilities in computation, atom-precise synthesis, and functional imaging converge.

The competitive scientific research program described in this Strategic Plan both contributes to and benefits from the collaboration with a vibrant user community. Although this community is largely from academia, CNMS will continue to improve outreach to *industry partners*, primarily by helping them understand how to frame and investigate the basic, publicly reportable scientific principles that underpin the challenges faced by industrial users. We will explore alternative cooperative mechanisms such as cooperative research and development agreements and promote CNMS capabilities effectively through industry outreach activities organized in cooperation with applied research programs at ORNL, in which industry contacts are very well developed.

In a continued effort to renew and reinvigorate in-house research, CNMS staff members are strongly encouraged to aggressively pursue funding from ORNL LDRD funds and to focus those efforts on projects that will lead to the development of new capabilities benefitting both in-house and user research. Partner user agreements, in which a user commits to the development of a capability at the CNMS, will continue to be strongly encouraged.

As our strategic vision indicates, the next five years will see that CNMS pursues a broad scientific agenda for energy and materials sciences in a close and dynamic collaboration with its user community, focusing on *understanding and controlling the complexity of electronic, ionic and molecular behavior at the nanoscale to enable design of new functional nanomaterials*. In-house research is well described within the three research themes; but those themes are expected (and designed) to evolve over time to address new opportunities, maintaining the focus on nanoscience that relates to novel energy technologies, i.e., on harnessing energy through nanoscience. With its specific combination of nanoscience capabilities leveraging powerfully on the neutron scattering and computing capabilities at ORNL, and its commitment to the development of new tools and methods for synthesis, theory/modeling, and characterization, CNMS is well positioned to advance this agenda at the forefront of nanoscience.

## List of Abbreviations

CNMS	Center for Nanophase Materials Sciences
APT	Atom-Probe Tomography
BASIS	Backscattering Spectrometer
CPN	Collective Phenomena in Nanophases
DOE	Department of Energy
EELS	Electron Energy Loss Spectroscopy
EIFN	Electronic and Ionic Functionality on the Nanoscale
FPHA	Functional Polymer and Hybrid Architectures
HFIR	High Flux Isotope Reactor
HIM	He-ion Microscopy
IFIM	Institution for Functional Imaging of Materials
LDRD	Laboratory Directed Research and Development
MAC-STEM	Monochromated Aberration-Corrected
NOMAD	Nanoscale-Ordered Materials Diffractometer
NTI	Nanomaterials Theory Institute
OLCF	Oak Ridge Leadership Computing Facility
ORNL	Oak Ridge National Lab
POWGEN	Powder Diffractometer
SEM	Scanning Electron Microscope
SEMPA	Scanning Electron Microscopy with Polarization Analysis
ShaRE	Shared Research Equipment User Program
SNS	Spallation Neutron Source
SPM	Scanning Probe Microscopy
SQUID	Superconducting Quantum Interference Device
STEM	Scanning Transmission Electron Microscopy
STM	Scanning Tunneling Potentiometry
TEM	Transmission Electron Microscopy
TMD	Transition Metal Dichalcogenides
UEC	User Executive Committee
VISION	Vibrational Neutron Spectrometer
VULCAN	Engineering Materials Diffractometer

