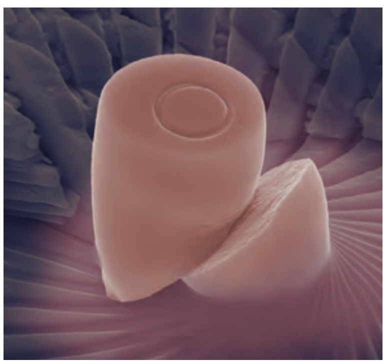
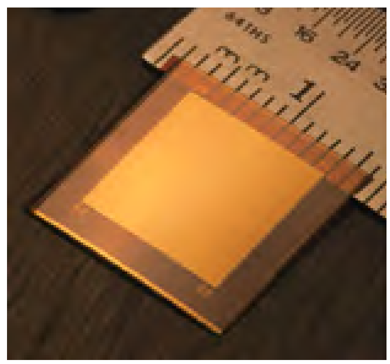
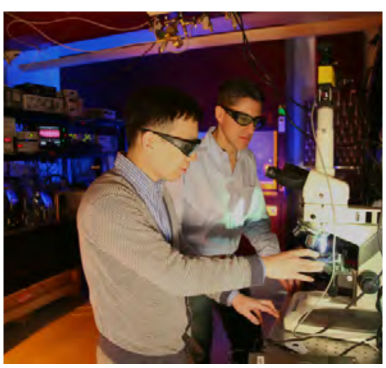
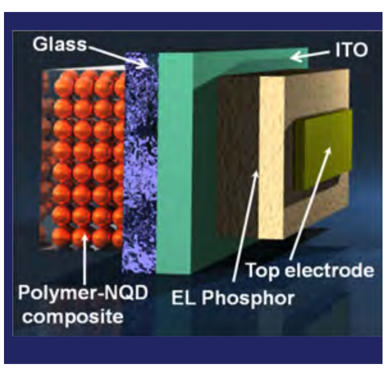
Los Alamos National Laboratory
Sandia National Laboratories

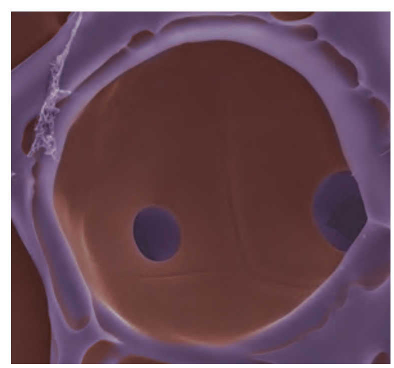
CINT 2020

The Center for Integrated Nanotechnologies Strategic Plan





LA-UR-14-25788

U.S. Department of Energy Office of Science

CINT Mission

The Center for Integrated Nanotechnologies (CINT) is a Department of Energy, Office of Science Nanoscale Science Research Center, operating as a national user facility devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials and structures. Through our Core Facility in Albuquerque and Gateway to Los Alamos Facility, CINT provides access to *scientific expertise* and *advanced capabilities* for researchers to create, characterize, understand and integrate nanostructured materials into the microscopic and macroscopic worlds. This comprehensive approach provides the greatest potential for nanostructured materials to inspire technological innovation with enduring beneficial impact in energy, environment, human health and security.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. Los Alamos National Laboratory, an affirmative action equal opportunity employer, is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.

Executive Summary

The Center for Integrated Nanotechnologies (CINT) plays a leadership role in the area of integration science through its function as a Department of Energy/Office of Science Nanoscale Science Research Center (NSRC) national user facility. By creating a collaborative community of diverse users matched to expert facility scientists with advanced capabilities, CINT fosters high-impact nanoscience discoveries, leads next-generation technique development and advances the frontiers of knowledge beyond that which is achievable by individual researchers or any single institution.

Deriving the ultimate benefit from nanoscience will require the assembly of diverse nanoscale materials across multiple length scales to design and achieve new properties and functionality; in other words, nanomaterials integration. Integration has played a pivotal and revolutionary role in the development of nearly all science and technology and is the overarching theme of CINT. Our strategic plan is based upon the extraordinary scientific opportunities involving nanomaterials integration in five challenges inspired by CINT users and our staff. Solving challenges such as these would unlock great possibilities for innovative technologies and have widely recognized impact in nationally important areas such as energy, environment, human health and security.

CINT's role is to enable world-leading science towards realizing these benefits and our strategic objectives describe what is needed to deliver on this promise. As a vibrant partnership between Los Alamos National Laboratory (LANL) and Sandia National Laboratories (SNL), CINT leverages the unmatched scientific and engineering expertise of our host DOE Laboratories in an Office of Science open-access user facility to benefit hundreds of researchers annually. We have world-leading *scientific expertise* in four thrust areas, as described in section 1, and *specialized capabilities* to create, characterize and understand nanomaterials in increasingly complex integrated environments.

Building upon these current strengths, we identify some of the capabilities and expertise that the nanoscience community will need in the future and that CINT is well positioned to develop and offer as a user facility. These include an expanding portfolio of our signature Discovery Platforms that can be used alone or as sophisticated "experiments within an experiment"; novel synthetic approaches for exquisitely heterostructured nanowires, nanoparticles and quasi-two-dimensional materials; ultra-high resolution spectroscopic techniques of nanomaterial dynamics; *in situ* microscopies that provide real-time, spatially-resolved structure/property information for increasingly complex materials systems; advanced simulation techniques for integrated nanomaterials; and multi-scale theory for interfaces and dynamics.

CINT's transformational and supporting foundational capabilities are made available to the widest possible number of qualified users via a comprehensive communications and outreach effort combined with an efficient user proposal, peer-review, and project management system. We will target research leaders in diverse institutions, early career scientists, and innovators in nanotechnology companies to create an expanded national user community of the future.

Finally, the CINT 2020 vision requires not only the prudent allocation of precious federal resources to support operations but also mutually beneficial new partnerships to bring state-of-the-art expertise and capabilities into the user facility of the future. We embark on this exciting journey ever mindful that the most significant metric of success is the quality of the science produced by the CINT community.

Contents

1.0 Introduction, Strategic Objectives and Organizational Alignment

The Center for Integrated Nanotechnologies (CINT) is a Department of Energy/Office of Science Nanoscale Science Research Center (NSRC) operating as national user facility. As a vibrant partnership between Los Alamos and Sandia national laboratories, CINT leverages the unmatched scientific and engineering expertise of our host DOE Laboratories to create a unique user facility environment among the NSRCs. Our users and staff conduct research projects within and across the *Core Facility* in Albuquerque, NM, and the *Gateway Facility* in Los Alamos, NM. By creating a collaborative community of diverse users matched to expert facility scientists with advanced capabilities, CINT fosters high-impact nanoscience discoveries, leads next-generation technique development and advances the frontiers of knowledge beyond that which is achievable by individual researchers or any single institution.

Thus our overarching goal:

CINT will be the national resource for *research expertise* and *advanced capabilities* to create, characterize, understand and ***integrate*** nanostructured materials in order to achieve unprecedented materials functionality and inspire revolutionary nanotechnologies.

In order to achieve this goal, CINT has the following six strategic objectives:

1. CINT will be the nationally recognized leader in nanomaterials integration.
2. CINT will develop unique experimental and theoretical capabilities to create, characterize, and understand nanoscale materials in *increasing complex integrated environments*.
3. CINT will develop next generation Discovery Platforms™ inspired by nanoscience integration challenges and will seek to proliferate the use of Discovery Platforms™ at user facilities and other institutions nationwide.
4. CINT will recapitalize to provide foundational capabilities and commercial instrumentation necessary for internationally competitive nanoscience research.
5. CINT will operate safely and effectively by aligning capability capacity with the ever-evolving user demand.
6. CINT will increase the diversity and breadth of our national user community, foster high-impact science, and encourage intellectual risk in basic and use-inspired research.

Together, these CINT strategic objectives support and align with the U. S. Department of Energy's Strategic Plan 2014-2018. Specifically:

DOE Strategic Objective 3 – Deliver the scientific discoveries and major scientific tools that transform our understanding of nature and strengthen the connection between advances in fundamental science and technology innovation.

In order to accomplish DOE Strategic Objective 3, the Department of Energy has three strategies, each of which is supported by CINT:

1. Conduct discovery-focused research to increase our understanding of matter, materials and their properties through partnerships with universities, national laboratories, and industry.
2. Provide the nation's researchers with world-class scientific user facilities that enable mission-focused research and advance scientific discovery.
3. Use the national laboratory system and leverage partnerships with universities and industry to conduct mission-focused research.

CINT is already implementing the three DOE strategies above. We have world-leading *scientific expertise* in and *specialized capabilities* to create, characterize and understand nanomaterials in increasingly complex integrated environments. Our expertise is organized in four scientific thrust areas:

- *Nanophotonics & Optical Nanomaterials* - Synthesis, excitation and energy transformations of optically active nanomaterials and collective or emergent electromagnetic phenomena (plasmonics, metamaterials, photonic lattices).
- *Nanoscale Electronics & Mechanics* - Control of electronic transport and wave functions, and mechanical coupling and properties using nanomaterials and integrated structures.
- *Soft, Biological & Composite Nanomaterials* - Solution-based materials synthesis and assembly of soft, composite and artificial bio-mimetic nanosystems.
- *Theory & Simulation of Nanoscale Phenomena* - Assembly, interfacial interactions, and emergent properties of nanoscale systems, including their electronic, magnetic, and optical properties.

In addition, we leverage the strengths of our host DOE laboratories through the alignment of the CINT 2020 strategic plan with the LANL and SNL missions, capabilities and strategic investments. For example, through the exploration of materials and integration, we support the LANL "Materials for Future of Los Alamos" scientific pillar which seeks to establish the design principles, synthesis pathways, and manufacturing processes for advanced and new materials to intentionally control functionality relevant to national security missions. Similarly, the SNL Strategic Plan includes explicit objectives in support of the nanoscience capability, materials science research foundation, and multiple crosscutting research challenges involving the creation, understanding and integration of advanced nanomaterials in technologies for national security applications.

The coordination of SNL, LANL and CINT strategic plans leads to very visible benefits for all three entities. Researchers from LANL and SNL continuously request access to CINT's capabilities and expertise through User project collaborations. Over the past three years CINT has hosted over 150 host facility researchers annually at the facilities, reinforcing the message that the laboratories value our Center, and that CINT closely partners with its host institutions to deliver high impact contributions to the labs core missions. These host laboratory projects are funded by a wide variety of sponsors including, but not limited to, The Department of Energy (including LDRD), The Department of Defense, The National Science Foundation, Homeland Security and The National Institutes of Health.

The exemplary science that comes from the CINT staff and collaborations with host lab and external users has received recognition by renowned sources. Most notably, CINT has won three R&D 100 awards in recent years. The R&D 100 Awards identify and celebrate the top technology products of the year spanning industry, academia, and government-sponsored research. Our R&D 100 winners include; 2008 – Tracking 3D Microscope (Werner, Goodwin), 2011 - Nanocluster Beacons (Yeh, Sharma, Martinez, Werner), and 2014 - Nano-Enabled, Microfluidic Detection of *Bacillus anthracis* (Harper, Bachand). These achievements illustrate the ever-growing potential for CINT to amplify the exceptional nanoscience strengths of our host DOE laboratories.

Finally, we note the special role that the DOE Office of Science user facilities have in supporting key objectives in 2014 National Nanotechnology Initiative Strategic Plan:

3.3. Provide, facilitate the sharing of, and sustain the physical R&D infrastructure, notably user facilities and cooperative research centers.

> 3.3.1. Establish regular mechanisms to determine the current and future infrastructure needs of users and stakeholders of these facilities and centers.
>
> 3.3.2. Develop, operate, and sustain advanced tools, infrastructure, and user facilities (including ongoing investment, staffing, and upgrades).

Nanomaterials integration is key to numerous extraordinary scientific challenges. Solving such challenges would unlock great possibilities for innovative technologies and have widely recognized impact in Nationally important areas such as energy, environment, human health and security. We describe five representative challenges in section 2, followed by the requisite expertise and capability development in sections 3 and 4, respectively. We also see new opportunities to refine the role of a user facility to meet the needs of a highly networked, international community.

Our vision for CINT in the year 2020, the six strategic objectives that are the pathway to achieving the vision, and dedication to continued excellence as a DOE Office of Science scientific user facility ensure that CINT will transform our understanding of nature and strengthen the connection between advances in fundamental science and technology innovation.

2.0 Science Vision: Challenges in Nanomaterials Integration

Nanoscale materials exhibit extraordinary physical, chemical, and/or biological properties. Isolated, or individual, nanoscale materials are scientifically interesting, but they rarely make significant technological impact. Building blocks comprised of individual nanoscale materials are commonly integrated with other materials into architectures that amplify their properties (up-scaling) or lead to new ensemble behaviors (emergent phenomena). By surveying the integrated environments of greatest potential impact, and by developing a fundamental understanding of the principles that govern the integrated properties and behaviors, we can capitalize on the greatest potential for nanomaterials to have an enduring impact on scientific and technological innovations. Nanoscale integration has the potential to revolutionize the way we live, in the same way that the development of the semiconductor-based integrated circuit (or computer "chip") did. The development of the "chip" required the capability to integrate a large number of resistors, capacitors, diodes, and transistors on a single platform. Once the "chip" was developed, it enabled countless innovations. CINT envisions similarly transformational technologies will ultimately emerge from nanomaterials integration.

Understanding the principles of nanomaterials integration has been the central theme of CINT since its inception. The CINT 2020 Strategic Plan builds upon this foundation by illustrating five representative, forward-looking integration challenges inspired by the nanoscience community. These integration challenges enable us to identify the capabilities that the nanoscience research community will need to realize the smart integration of nanomaterials into innovative and competitive technologies. To accomplish these challenges, CINT will bring together expertise and capabilities across our four Science Thrusts. An underlying theme of all five challenges is a fully integrated feedback loop of synthesis, characterization, and modeling, shown in Figure 1 (also described in more detail on the NSRC Portal) that will allow the nanoscience community to realize, and develop the ability to predict and a priori design, unprecedented materials functionalities.

Figure 1. CINT leverages its diverse scientific community to fully integrate theory and experiment.

2.1 Nanofabrication and nanoepitaxy for arbitrary multifunctional quantum semiconductor structures and their assemblies

In recent years, substantial improvements have been made in techniques to fabricate, grow, and understand nanomaterials with desired electronic and optoelectronic properties. These materials could lead to future innovation for energy-efficient "light capture" (e.g., solar energy, light/radiation detection) and "light emission" (e.g., solid state lighting, quantum communication).

CINT is already at the frontier of these research areas, and is perfectly poised to fundamentally advance the field. CINT has state-of-the-art capabilities in molecular beam epitaxy (MBE) growth (see photo) of high-mobility III-V planar heterostructures and bottom-up chemical vapor deposition (CVD) synthesis of group IV nanowires. CINT also has a 9,000ft^2 clean room facility with processing tools that can reach a resolution of tens of nanometers. Traditionally, nanomaterial system fabrication has been carried out in planar structures (Figure 2a). More recently, however, 3D architectures have started to emerge in silicon electronics (Figures 2b and 3). The translation of these structures to three dimensions (Figure 2c) will ultimately expand their utility to many technologies including consumer electronics, energy, and biomedicine. However, this will require substantial innovation in the nanofabrication, growth, and integration of quantum-size structures.

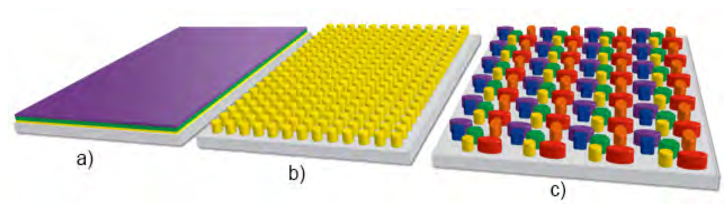


Figure 2. a) Thin films, (b) a homogeneous nanowire array, and (c) an hypothetical device based on heterogeneous nanoscale integration of dissimilar structures.

Combinations of bottom-up and top-down growth and nanofabrication techniques have been used successfully to create “vertical” nanowires in a few material systems such as group IV and certain III-V semiconductors as shown in Figures 2b and 3. In a way, nanowires represent a very simple 3D architecture where carriers can be confined along one or two dimensions. More complex 3D structures that contain a variety of semiconductors with sections of varying dimensional confinement (1D, 2D & 3D) are required for new applications such as low threshold lasers, quantum information and computation, new transistor architectures that go beyond the semiconductor roadmap, and novel optomechanical systems. Hybrid multi-sequential combinations of bottom-up and top-down synthesis techniques must be developed in a variety of combined semiconductor families, possibly oxides or diamond, to realize this vision. One hypothetical example of an application where heterogeneous integration of dissimilar structures and materials could be used is single-photon sources for quantum information processing. An ideal single-photon-on-demand source could be made from an electrically injected quantum dot. To accomplish this, a nanodevice would have to be made from different direct bandgap III-V semiconductors emitting at different wavelengths. The semiconductors would have be placed in specific locations in a 3D arrangement for subsequent coupling to passive waveguides made from group IV semiconductors for further multiplexing and routing. Developing architectures such as this will require the integration of different dimensional structures into a larger functional microstructure as shown in Figure 2c. CINT will move this, and other, notional nanomaterials closer to reality by systematically addressing the following scientific questions:

- Can new nanofabrication and growth routes be devised to create new structures that contain vertical or horizontal quantum wires, individually or connected in networks? Or assemblies of nanofabricated quantum dots (free-standing or embedded in nanocavities)?
- Can wrapped gated 3D transport devices be devised using novel growth combined with fabrication for quantum transport studies?
- How can 3D suspended elastic structures, hybrid photonic/phononic/electromechanical lattices, and similar devices be created? All these nanostructures could be further assembled or integrated into a higher mesoscale hierarchy to produce new collective behaviors.

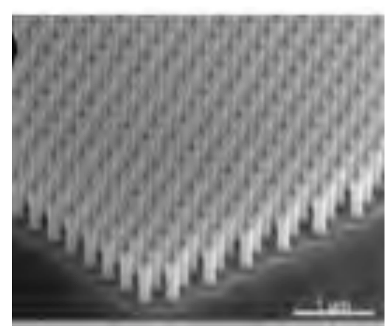


Figure 3. Nanowire arrays.

- How can the theory of some of these new mesoscale assemblies (combined optical, mechanical and transport) be developed?

To address these questions, CINT hopes to expand its growth capabilities into other semiconductor families such as large band gap semiconductors (i.e., III-Nitrides, diamond) and low band gap materials (e.g., InGaAs/InP, antimonides), and expand the MBE effort into high-mobility group IV materials. The integration of different semiconductor materials laterally and vertically, as shown in Figure 2c, will necessitate the development of new hybrid growth techniques with *in situ* sample handling and characterization in vacuum, all combined with new nanofabrication techniques. In addition to the expansion and combination of epitaxial capabilities, new nanofabrication techniques must be developed to create arbitrary top down nanostructures that go beyond "vertical etching". CINT researchers envision the capability to create quantum wires that lie horizontally in several planes, and with arbitrary control of their diameters and connectivity to other top-down or bottom-up defined sections.

These new experimental efforts will stimulate new, associated theoretical efforts. CINT will leverage our integrated synthesis, characterization, and modeling capabilities (Figure 1) to better understand areas such as combined electronic, optical, mechanic and electromagnetic behavior in multi-dimensional semiconductor structures.

2.2 Scaling one-dimensional nanostructures for macroscale relevance

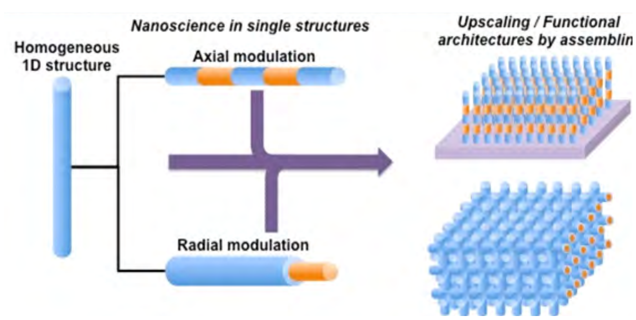


Figure 4. Scaling 1D nanostructures for macroscale relevance

Semiconductor nanowires and nanotubes are important building blocks for next-generation energy-harvesting and energy-storage systems, optoelectronics (from single-photon sources to low-threshold lasers), photodetectors, and even sensors for chemical or biological agents. Significant progress has been made in recent years in the precision synthesis of single-crystalline, controllably doped, and heterostructured (both radially and axially) nanowires, as well as in the selective preparation of nanotubes with specified structure and chirality. Furthermore, probes have been developed that have made it possible to determine electrical, optical, and thermal properties at the level of a single nanowire or nanotube, and even physically manipulate single wires. However, one of the biggest challenges in nanowire science is how to up-scale and organize structures and architectures into ensemble systems that are functionally relevant as shown in Figure 4.

"Upscaling" nanoscale thermoelectrics: The challenge of scale is especially relevant to nano-enabled thermoelectrics (TEs). In contrast with other potential nano-enabled technologies (lighting, sensing, solar energy harvesting/storage), thermoelectricss require bulk-scale assemblies to achieve high efficiencies at the up-scale level (that is, the cm scale, rather than nm – μm scale). This requirement remains a key challenge to translating nano-properties to technologically relevant efficiencies. CINT will work to overcome the issues currently associated with upscaling by addressing the following questions:

- Is it possible to bridge the physical gap between emergent nanoscale functionality and macroscale performance requirements? If 'building block' nanomaterials are to be used to create functional systems from the bottom up, such as interconnected networks or composite mesoscale structures, how will interface effects be managed?

- Can new concepts for coupled hybrid materials systems provide the framework for realizing multi-functionality in the case of combined structural functionality (structural integrity, facile handling, device integration) and an optimized nano-derived figure-of-merit? Is “up-scaling” compatible with conventional device architectures?
- Can multi-scale modeling guide the development of thermoelectric devices full cycle, from nanomaterials optimization through integration and device design?

Paradigm change in nanowire optoelectronic design: Optoelectronic systems require excellent photon manipulation and efficient photo-generated carrier transport. For instance, nanowires conceptually provide novel opportunities to achieve almost perfect light absorption in the solar spectrum as well as ultrafast carrier collection for photovoltaics. But useful performances of nanowire systems originate from integrated nanowires, rather than a single nanowire. The relationship between scaling nanowire arrays and light absorption properties has been elucidated thoroughly in the last decade. However, integration of nanowire arrays in electrically driven circuits requires novel processing developments since these nanostructures are inherently based on three-dimensional architectures with multiple heights. Such a large depth of field cannot be processed with current lithographic techniques. Additionally, the multi-scale architecture – encompassing the spacing between nanowires at the nanoscale and sizes of integrated light absorbers (nanowire p-n junctions) at the meso or microscale – makes the process difficult since current semiconductor processing has been optimized for high throughput at a different scale. Complementarity to lithographic-based systems will need to meet the scaling challenges inherent to solution processing of nanowires and nanotubes. A primary challenge in solution-based optoelectronic films is that transport is often limited by hopping and/or percolation mechanisms. A mesoscale strategy must start at the fundamental element level, and encompass mid-range interactions to the large-scale behavior of the system. CINT will explore ways to bridge these scales by addressing the following questions:

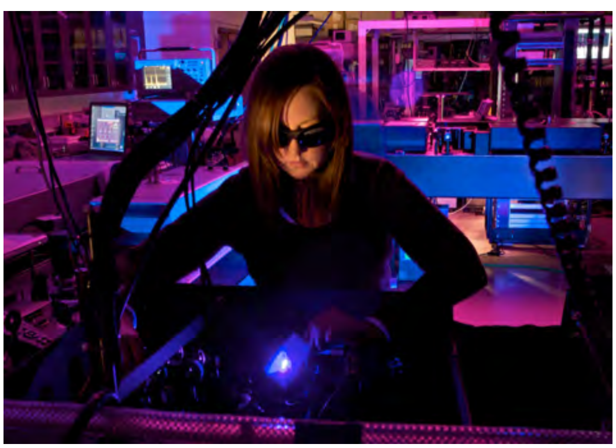
- Can interaction geometries and film architectures be devised that harness the exceptional axial diffusion behaviors of 1-D systems?
- Can solution chemistry (including self-assembly, surface chemistry, and novel film processing techniques) be used to create tailored assemblies in which pre-designed morphologies define the interfacial behaviors that control energy and charge flow? Can the new photophysical responses that we introduce via doping or functionalization at the nanoscale into single isolated elements be modified or enhanced through interactions in small-scale aggregates or clusters of elements? Can such emergent behaviors be predicted and harnessed at the meso- and macroscale?

Organizing nanostructures into mesoscale architectures for electrical energy storage: Regular arrays of nanowires have been used to study electron and ion transport at the nanoscale for battery applications. In pursuit of higher capacity, higher power, and efficient capacity retention for rechargeable batteries, complicated mesostructures composed of nanostructures such as ‘nanowire forests’ and ‘woodpile-like multi-stacks' have been suggested for battery architectures. One of the most important features of mesoscale architectures is that they are neither ordered nor completely random; they are best categorized as fractal. Porosity and tortuosity are key parameters in correlation with energy and power density. CINT will seek to better understand and ultimately control these complex meso-architectures by investigating these, and other related, questions:

- How can complex, desired nanowire structures be assembled?
- What are the ion or electron transport behaviors at the junctions of nanostructures?
- How can structures that are neither ordered nor random be modeled and characterized?

CINT is well positioned to address all these questions by leveraging established capabilities in nanowire and nanotube synthesis and chemical modification, nano-manipulation for direct measurement of a nanostructure's properties, and fabrication of single nanowire devices. CINT's Discovery Platforms for thermoelectric and electrical characterization and *in situ* TEM measurements of transport and electrochemical processes in single nanowires have also enabled many discoveries in this area, and will be applied and expanded to meet these challenges. The expansion will require developing unprecedented capabilities in multi-scale characterization, including integrating wide field observation with nano- and mesoscale resolution in up-scaled three-dimensional architectures. CINT has already demonstrated the application of ultrafast wide field optical microscopy for multi-scale characterization, and will expand its multi-scale probing capabilities in other physical characterizations. CINT will also leverage our integrated synthesis, characterization, and modeling capabilities (Figure 1) to better understand the phenomema that underlie these architectures.

2.3 Hybrid material interactions for generation and manipulation of light



In recent years, there has been increasing interest in the creation of hybrid systems. Exactingly structured hybrid materials can be engineered to have novel properties that don't occur in nature, including pre-designed properties for novel photon generation and manipulation characteristics. CINT aspires to advance the understanding and application of these revolutionary hybrid systems by addressing the most significant open questions surrounding the control, integration, and enhancement of the response of two classes of materials and their associated assemblies:

- Materials that control and modify electromagnetic energy (plasmonics, metamaterials); and
- Materials that actively generate and harvest electromagnetic energy.

Generation and active manipulation of novel emitting states and photon correlation statistics: Accessing new emission regimes of expanded wavelengths, enhanced quantum yields, and tunable or selectable photon statistics and dynamics requires defining interactions in terms of the relative placement and orientation of materials within the hybrid structure, while also controlling the hybrid composition over multiple dimensionalities. CINT will expand the hybrid materials community's ability to generate and actively manipulate novel emitting states and photon correlation statistics by addressing the following questions:

- How can candidate materials that are likely to generate targeted optical behaviors from hybrid interactions be identified?
- How can multi-component systems with the appropriate interaction geometries to create a desired functionality be best synthesized and/or integrated?
- How can emergent electronic structures be manipulated and probed across multiple length-scales within interfacial environments to generate desired optical responses?

CINT will employ a variety of materials processing techniques, including direct synthesis, self-assembly, nanofabrication and directed placement, to further our understanding of these issues. CINT will also move beyond traditional synthetic and processing approaches by tapping soft-materials assembly methods with the potential to harness the responsive and highly tunable nature of bio-inspired systems.

Active, multifunctional plasmonic and metamaterial interactions: Hybrid materials interactions have significant potential for establishing new functionality and enhanced manipulation of the medium in which light is generated, harvested, or propagated. Hybrids enable a move from passive to active plasmonic and metamaterials, and form a basis for new concepts including metamolecules (in which the collective interactions of individual metamaterial elements or atoms create new function) and "plasmonics on demand" (where localized materials interactions automatically generate desired resonances in optimized locations). Unprecedented multifunctionality will result, giving simultaneous control of polarization states, beam steering, and focusing; integrating perfect absorption of light directly into optoelectronic architectures; or ultimately integrating hybrid metatmaterials directly with emerging concepts in emitting materials. To realize this extraordinary multifunctionality, CINT will utilize our integrated efforts in synthesis, characterization, and modeling (Figure 1) to address the following questions:

- What can be achieved with non-traditional plasmonic systems (e.g., graphene hybrids) that cannot be accessed with more traditional noble metal approaches?
- Can multifunctional metamaterial behaviors be designed through metamolecule concepts (shown in Figure 5)?
- How can hybrid interactions coupled to metamaterials architectures be used for active/dynamic control and tuning of enhanced metamaterial response?

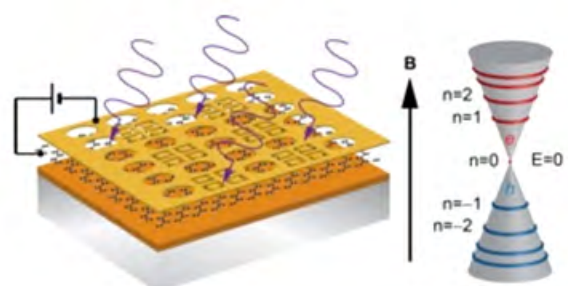


Figure 5. Integrated meta-molecule based metamaterials.

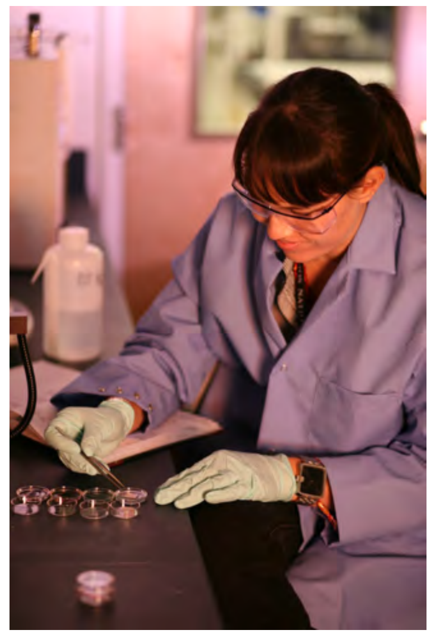
Meeting the modeling challenge: CINT's ultimate goal in this area is to create hybrid materials by design. This will entail significant advances in predictive modeling. In particular, the state-of-the-art must be dramatically advanced in such areas as electronic structure, dynamics, environment, and interfacial interactions at length-scales between the molecular and macroscopic. To meet the modeling challenge, CINT will address the following questions:

- How can a predictive capability to understand and anticipate new optical functionality arising from materials interactions be developed?
- What materials interactions, both in terms of composition and interaction geometries, are most interesting and promising to pursue as routes to novel optical behaviors?

- What new theoretical concepts must be developed to access the middle-length scales of significance to understand integrated hybrid behaviors?

CINT's current expertise and capabilities in hybrid materials provide a strong foundation for pursuing the above questions However, the full range of effort in this area will require CINT to expand its materials generation capability to include new techniques capable of placement of optical nanoparticles with nm precision. Additionally, our strengths in single-nanoparticle spectroscopic characterization could be significantly enhanced by adding capability for single nano-element Raman and magneto-optical spectroscopy while expanding ultrafast capabilities to include single-photon counting techniques at wavelengths longer than the near-IR. CINT will also bring the full strength of our integrated efforts in synthesis, characterization, and modeling (Figure 1) to bear on these issues. Model development will work hand-in-hand with experiment in this rapidly expanding field, to allow us to establish the most relevant model systems for validation of predictive models.

2.4 Multi-scale structure and dynamics in soft matter



The ability to a priori design and create multi-scale, dynamic soft materials and composites that are capable of adaptively sensing and responding to their environment, controlling energy flow, and processing information is an important grand challenge in nanomaterials science. The plasma membrane of a cell is an excellent example of such a material. The membrane plays a central role in a wide variety of complex physiological functions, including signal transduction (the ability to sense a change in the external environment and trigger a chemical response inside the cell). The functionality of these membranes is strongly dependent on the dynamic, multi-scale organization of the individual molecules that comprise it. While the properties of synthetic and composite materials can be achieved by doping with nanoparticles and regulated by adjusting particle morphology, these materials presently lack the ability to perform complex and elegant functions like those of biological systems.

Development of soft nanomaterials with complex functionality is currently limited by a lack of guiding principles that allow for the rational selection of molecular constituents and means by which to combine them effectively into dynamic, multi-scale materials with the desired functionality. CINT will fundamentally advance our understanding and ability to exploit the properties of soft materials through a convergence of numerical simulations and experiments, which will enable the ability to characterize and understand dynamics across multiple length and time scales. Achieving this will require CINT to address the following questions:

- How do we couple disparate, multiple nanoscale objects to create functional, hierarchically structured composites?
- How do we design and develop interfaces capable of responsive reorganization while also enabling multiscale integration?
- How do we design and implement interfaces that promote efficient transport (energy and information flow) between coupled entities?

When combining multiple molecular or nanoscale constituents to generate hierarchically structured materials or composites, interfaces become increasingly important: the interface must be dynamically responsive in order to couple the critical components that produce macroscale functionality. To address the three questions above, CINT will push the state-of-the-science beyond simple homogeneous building blocks as shown in Figure 6a, and instead create building blocks with multiple or combined structure and/or chemical functionalities as shown in Figure 6b. Moreover, producing complex behaviors that bridge multiple length scales requires a transition from static to responsive and/or programmable interfaces in which dynamic interactions drive structural reorganization and associated changes in function. Integration of these new, complex building blocks into a mesoscale assembly, like that shown in Figure 6c, is another key element for materials development that will be advanced using CINT's integrated synthesis, characterization, and modeling approach (Figure 1).

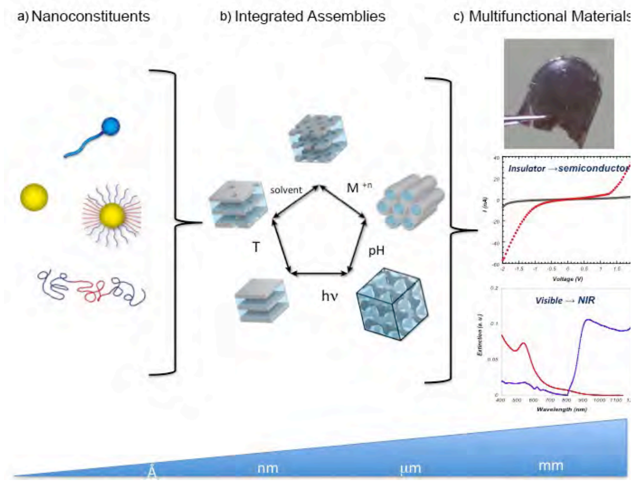


Figure 6. Bridge nanoscale and macroscale

Development of soft nanomaterials with complex functionality will require substantial improvements in techniques for the simultaneous *in situ* characterization of multi-length scale *and* temporal phenomena. In recent years, considerable progress in optical microscopy has enabled characterization of soft and biological materials with spatial resolution well below optical diffraction limits, and with high temporal resolution. While these techniques are well suited for evaluating the interfacial dynamics of individual nanoscale components, they often lack the ability to capture details of the molecular structure of complex assemblies. Understanding these molecular assemblies is key to understanding both interface properties and macroscale functionality.

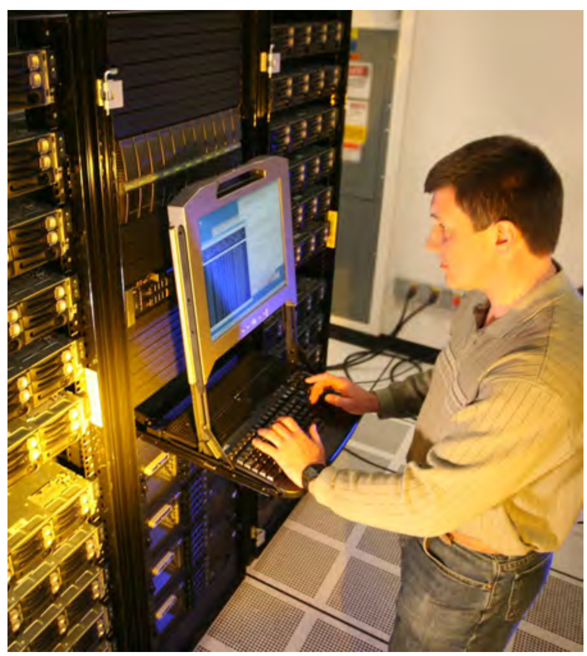
In contrast, techniques such as electron microscopy (e.g., cryo-TEM), and neutron and x-ray scattering allow for high-resolution imaging of complex materials over a wide range of length scales (Å – mm), but do not readily probe dynamics at relevant timescales. Thus, the integration of multiple techniques to create multi-modal analysis is a key opportunity for nanoscience research. Toward this end, CINT has already developed novel high-resolution optical imaging techniques (e.g., 3D tracking and super-resolution optical spectroscopy) for monitoring the dynamics of nanoscale objects (e.g., nanoparticles, proteins) within soft matrices and composites. In the future, other techniques such as proximal probes, *in situ* TEM, and neutron and X-ray scattering, will be coupled in order to further our understanding of hierarchical soft materials. This ultimately will allow us to design, *a priori*, engineered composites. Ultimately, the integration of multi-modal structural and temporal characterization platforms could also be coupled with combinatorial synthetic platforms (e.g., Microfluidics Discovery Platform) to enable real-time, *in situ* visualization of multi-scale dynamics and assembly processes. CINT will work to make emerging approaches, such as these, a reality. This will allow an unprecedented level of insight into interfacial structure and dynamics.

Along with the aforementioned improvements in experimental characterization methods, advances in high performance computing have resulted in an overlap of time scales and system sizes between atomistic simulations and experiments for some nanoparticle systems. The development of coarse-grained models from the underlying atomistic models is expanding the spatial and temporal ranges significantly, while maintaining key chemistry. CINT is perfectly poised to take advantage of these developments, which will be the key to the a priori design of multi-scale, dynamic soft materials and composites with engineered functionalities.

2.5 Theoretical modeling and first-principles simulations of multi-functionality in hybrid nanostructured systems

As discussed in Sections 2.1-2.4, significant advances in nanoscience and nanotechnologies have enabled precise fabrication of very small objects with unique electronic functionalities, including quantum dots and metal particles, macromolecular structures, chemically functionalized nanotubes and graphene structures, etc. At the same time, advances in high performance computing have resulted in an unprecedented ability to model these systems, and thereby understand the phenomena that contribute to their functionalities.

The reduced physical dimension and size of nanoscale systems heighten the importance of quantum effects, which enormously enriches the realm of emerging nanotechnologies. On the one hand, quantum mechanical first-principles approaches – developed over the past two decades – uncover the microscopic processes of electronic and optical phenomena at the nanoscale. On the other hand, there is increased interest in fabricating hybrid structures with these nanoscale building blocks toward technological applications. Furthermore, emergent phenomena intrinsic to strongly correlated electronic materials open a new opportunity toward multiple functionalities. These interesting phenomena pose significant challenges to theory, modeling, and simulation at the scale of macroscopic relevance. Ideally, theory should enable one to understand the fundamental processes responsible for the emergent behaviors and properties of these hybrid structures, enabling the prediction and control of novel functionality that cannot be achieved by "simple" bulk or single-phase nanomaterials. One of the biggest challenges in the theoretical modeling is to establish a coupled approach that is based on the closed synthesis-characterization-modeling loop, as schematically illustrated in Figure 1. CINT will leverage its ability to integrate theory and experiment to address questions raised in Sections 2.1-2.4, both to improve our understanding of the systems described in those sections, and to fundamentally advance nanomaterials integration.



For example, in the field of energy research, the ultimate goal of many researchers is to solve the global energy crisis by discovering a sustainable green technology that harvests unlimited, clean solar energy. One approach to solving this problem has been the assembly of nanoblocks into systems that collect light and transport energy and charges with minimal loss. However, energy transport is strongly modified in these hybrid structures. As the interactions among different degrees of freedom become stronger, composite excitations such as plasmons, excitons, polarons, and polaritons become important components of transport due to quantum correlations among different degrees of freedom. A unified description of these different degrees of freedom in a hybrid structure is a key challenge to theory in this area of research. CINT will explore solutions to this problem by addressing the following questions:

- What are the coupling mechanisms across interfaces between different nanoscale building blocks?
- What are the design principles that govern the conversion of optically generated excitonic excitations into electrical charges in hybrid structures for energy harvesting?
- How can the transport of energy (excitons) and charges in inherently amorphous materials be manipulated via synthetic control over the structure of buried interfaces and defects?

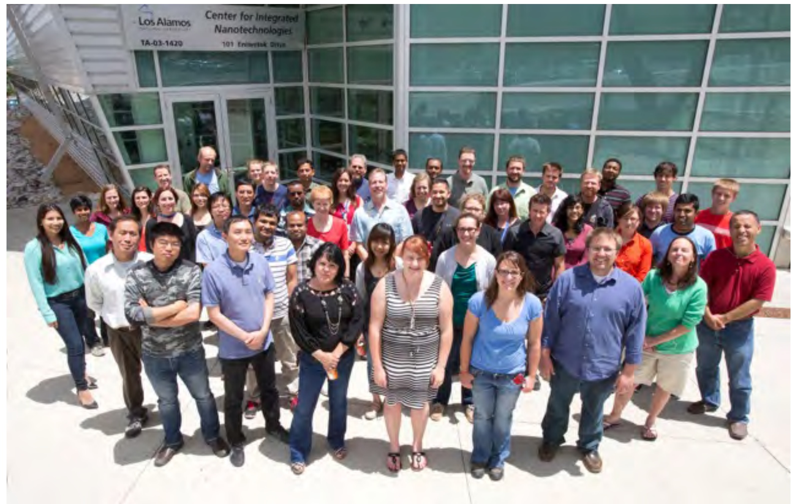
Another example is the emergent phenomena observed in correlated electronic materials. In the last few decades, novel classes of materials have been discovered in which competing interactions produce exotic and unexpected properties, including anti- and ferromagnetism, superconductivity, heavy fermion behavior, and multiferroics. These emergent phenomena, which are absent in semiconductors, have the potential to revolutionize our future energy and information technologies. More recently, new functionality of correlated electronic materials has also been demonstrated by the epitaxial growth of complex oxide multilayers or three-dimensional mesoscale structures. The key to these intriguing phenomena is the strong entanglement among spin, charge, orbital, and lattice degrees of freedom in the correlated electron materials. This complexity poses a significant challenge to modern condensed matter theory. In this frontier, there is no powerful theory for understanding and predictive design of improved functionality. CINT will seek to remedy this gap by addressing the following questions:

- What are the design principles that govern couplings in the competing degrees of freedom in hybrid/interfacial structures with electronic correlations?
- How can functionality be optimized by combining the intrinsic tunability of complex materials into hybrid architectures?
- How can microscopic interactions be tuned to produce precise control of the mesoscale functionality in hybrid structures?
- How does the nonequilibrium response of spin/charge/lattice degrees of freedom at the mesocale lead to controlled functionality?

The answers to these fundamental theoretical questions have relevance across Sections 2.1, 2.2, 2.3 and 2.4, and will be validated using CINT's immediate access to the same experimental synthesis and characterization capabilities that will be used to address the questions posed in those sections. On the other hand, the advances in theory produced by exploring these questions will support experiments defined by Sections 2.1 through 2.4 through interpretation and prediction.

3.0 Scientific Expertise to Realize the Vision

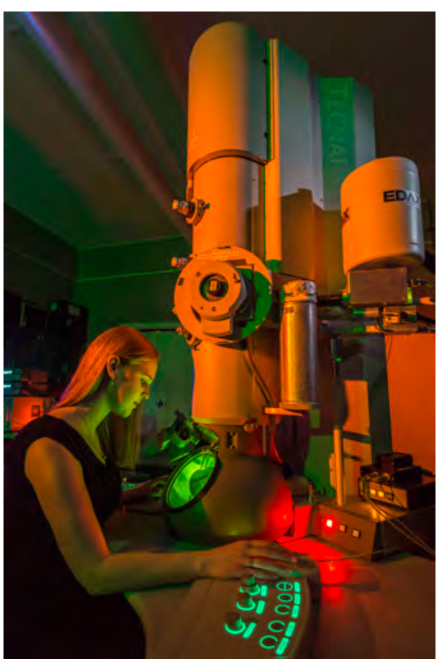
Nanomaterials integration involves:



1. synthesizing and fabricating individual nanoscale building blocks, which may be combined to form specific heterostructures,
2. characterizing their functionalities,
3. understanding their fundamental chemistry and physics,
4. assembling these building blocks, and
5. delivering a functional material system.

The fundamental challenges underlying such integration go beyond complex fabrication or the engineering of known solutions; they lead to novel discoveries and new sciences.

Currently, the four thrusts as described in Section 1 (namely Nanophotonics & Optical Nanomaterials, Nanoscale Electronics & Mechanics, Soft, Biological & Composite Nanomaterials, and Theory & Simulation of Nanoscale Phenomena) have already demonstrated their specific strengths and scientific expertise at the international level. A wide variety of activities is being initiated within the four thrusts and our user community, including research activities, user projects, new instrumentation, Discovery Platforms, and cross-thrust activities. These areas are being developed to be mutually supportive and to maximize their value to our user program and the scientific community. Our internationally recognized expertise in different scientific and technological fields has positioned ourselves in a leadership role in nanoscience research.



However, as both nanoscience programs and nanomaterials integration continue to evolve in response to new scientific challenges in the scientific community, we will need not only to retain our current workforce to maintain our forefront role in nanomaterials integration, but also to strategically hire more scientists with expertise in fields such as system level modeling, architecture designs, and in-situ multi-length scale/temporal characterization of soft materials to address the dynamic integration challenges and other challenges described in Section 2 to realize CINT's overall vision of nanoscience.

With our current and expanded expertise, we will maintain our leadership role in nanomaterials integration. Our scientists will continue to be actively engaging our user community through a variety of mechanisms to promote integration of nanomaterials as well as to address challenges in scientific frontiers.

4.0 Transformational and Foundational CINT Capabilities

Through a combination research expertise, specialized capabilities, and essential foundational techniques, CINT enables our users to perform complete research projects that would otherwise not be possible. Therefore, to address the research challenges of the future, CINT is continuously improving its current capabilities, exploring concepts that can lead to new experimental, theoretical and computational methods, and selectively disinvesting in capabilities that are no longer state-of-the-art.

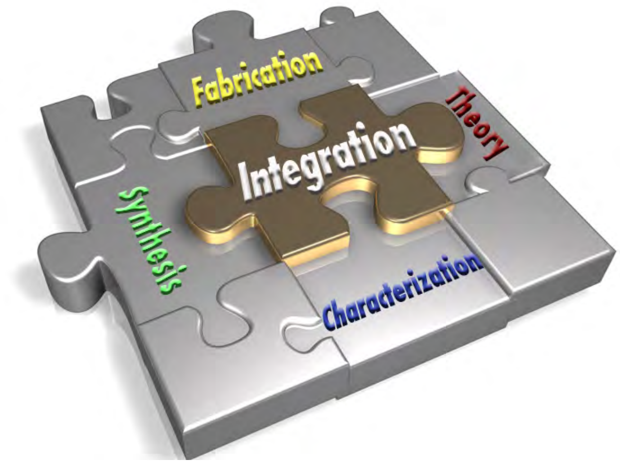


Figure 7. Addressing integration through collaborative capabilities and expertise in fabrication, synthesis, characterization and theory.

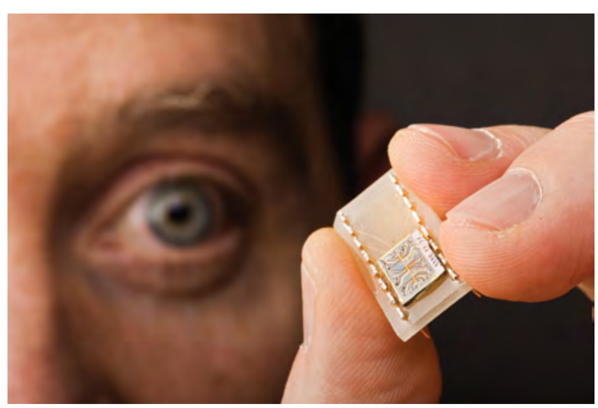
In this section, we identify a selection of CINT capabilities that will be important in addressing future integration challenges and that will transform the way integration research is conducted (CINT strategic objective 2). Some involve significant upgrades to current capabilities while others will require entirely new efforts that build on our expertise.

In addition to the specialized capabilities highlighted here, CINT has many more which form an essential foundation for the majority of nanoscience research. The complete list can be viewed on our website. As specified in CINT strategic objective 4, CINT must continue to recapitalize this infrastructure to have the baseline instruments that all researchers need to properly measure and control the relevant conditions in their experiments.

By virtue of having two DOE host laboratories, CINT is uniquely able to leverage a wide range of expertise plus substantial prior investment in research infrastructure. While there are several examples of this synergistic benefit in our capabilities as shown in Figure 7, perhaps the most differentiating among the DOE/SC user facilities is our portfolio of Discovery Platforms™.

4.1 Discovery Platforms: A CINT Signature Initiative

The need to reproducibly characterize individual nanostructures or synthesize nanomaterials with exquisite chemical control has inspired CINT to develop Discovery Platforms™. These unique research tools consist of micro-fabricated structures or devices for specific nanoscience experiments. Simple platforms are fabricated in CINT whereas the most complicated devices, essentially a lab-on-a-chip, are designed and produced in cooperation with the Microsystems Engineering Science and Applications (MESA) facility at Sandia National Laboratories.



Discovery Platforms are conceived, designed and commissioned with user input and active participation. They allow users to conduct experiments that are not possible using traditional laboratory equipment. The present suite of Discovery Platforms includes:

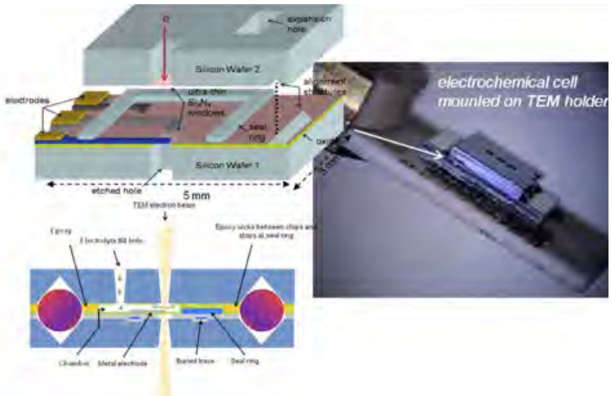


Figure 8. Electrochemical Discovery Platform.

Electrochemical Discovery Platform: The ElectroChem Discovery Platform is a microfabricated fluidic platform designed to study electrochemical energy storage processes in real time inside a transmission electron microscope as shown in Figure 8. This platform enables direct observations of solid/liquid interfacial process such as electrode/electrolyte interactions, electrode dissolution in electrolyte and solid-electrolyte interphase layer formation.

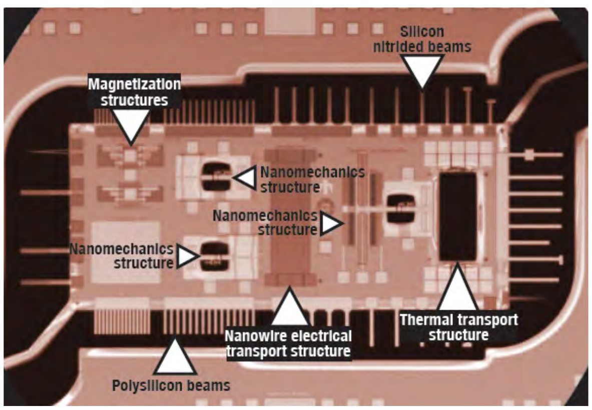


Figure 9. Nanomechanics and Thermal Transportl Discovery Platform.

Nanomechanics and Thermal Transport Discovery Platform: The goal of the CINT Nanomechanics and Thermal Transport Discovery Platform as shown in Figure 9 is to enable researchers to perform experiments related to nanomechanics, sensing, scanning probe microscopy, *in situ* TEM, and magnetization measurements, all using structures on a single, small chip-based platform. A new version of this Platform also includes structures for measurements of the electrical properties, thermal properties, electromechanical behavior, and microcalorimetry of nanoscale samples.

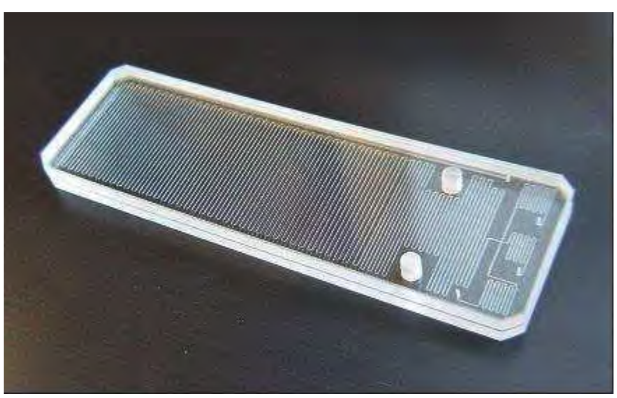


Figure 10. Microfluidics Discovery Platform.

Microfluidics Discovery Platform: The new Microfluidic Synthesis Discovery Platform as shown in Figure 10 is an extremely flexible system for nanoparticle synthesis, functionalization, and real-time characterization. The microfluidic system utilizes an all-glass chip with a serpentine channel that can hold volumes from 200 microliters to one milliliter and precision temperature control. Real time reaction monitoring via visible and fluorescence microscopy, as well as UV-vis spectroscopy are currently being used with IR spectroscopy and dynamic light scattering to be added in the future.

The integration science challenges present exciting new opportunities to develop next-generation versions of these Discovery Platforms™ and to invent additional platforms in conjunction with CINT users designed for the synthesis and characterization of integrated nanomaterial systems (CINT strategic objective 3). As with all platform design cycles, the intial step is to specify the specific desired functions of a new platform, the performance criteria, and the scope of research for which it is expected to be used. These early platform concepts are then vetted with the external scientific community via Discovery Platform Workshops and focused sessions at the annual CINT User Meeting.

A central issue in the development of multi-scale materials is large-scale predictive assembly of nanoscale building blocks (e.g., colloidal nanoparticles, polymers, proteins, etc.) into functional mesoscale assemblies. One approach to address this limitation is the development of experimental systems that can achieve reproducible synthesis and most importantly, assembly of the building blocks. Work in this area will build off of CINT's Microfluidic Discovery Platform™ and expand into more complex architectures that enable the rapid prototyping of molecular building blocks, as well as the controlled assembly of soft matter, particularly into 3D mesoscale assemblies. In new development, there will be a strong emphasis on integrating the Microfluidics platform with new capabilities and techniques developed as part of the in situ characterization effort, as described above. The key objective will be developing new Discovery Platforms that enable tight coupling of in situ characterization and microfluidic delivery that will enable real-time control over multi-scale, hierarchical assembly.

An important new direction for CINT will be collaborations with other Nanoscale Science Research Centers and DOE/SC user facilities (light sources and neutron scattering centers) to couple the capabilities of a Discovery Platform™ with unique instrumentation at these other national user facilities. The future outcome will be not only an expanding portfolio of platforms optimized for nanomaterials integration at CINT but also a wider community of researchers using these microscale instruments for other cutting edge research Nationwide.

4.2 Synthesis / Fabrication

Creating novel integrated nanomaterials requires robust methods to reproducibly synthesize nanoscale constituents with known composition and structure, rigorous control of assembly processes to organize the components ("bottom up assembly"), and microfabrication tools ("top down fabrication") to prepare architectures that connect nano-to-macro length scales. CINT currently offers and continuously develops these state-of-the-art capabilities including the following:

- By understanding the effects of shell thickness, core size, core/shell electronic structure, and internal nanoscale interface properties, we have developed non-blinking nanocrystal quantum dots that emit in the visible and the near-infrared. More broadly, CINT is pioneering approaches for optical nanomaterials by design.

- Working closely with physicists and theorists who inform our synthetic work, we pursue novel chemical-precursor and ligand/surfactant approaches to synthesize a wide variety of metallic/magnetic nanoparticles and fluorescent nanoclusters with unprecedented control over particle size-dispersity, crystallinity, stability and magnetic properties.

- CINT is integrating biomolecular components, such as motor proteins, to create responsive, multifunctional materials that

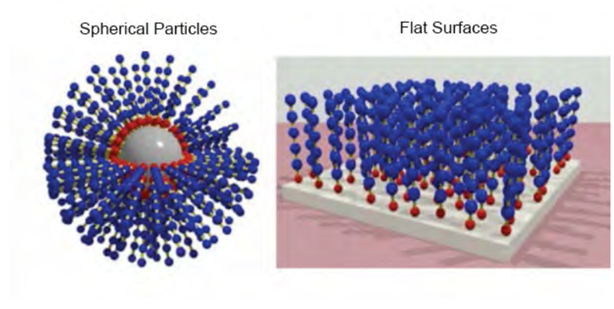


Figure 11. Schematic illustration of bioinspired functional composites

bridge the nano-bio worlds. We will build on current strengths to create hybrid nano-bio-materials, bioinspired functional composites (e.g., nanoparticle-polymer and nanoparticle-protein composites) as schematically illustrated in Figure 11, and biomimetic synthetic polymers with a strong emphasis on programmable and/or responsive materials.

- CINT specializes in the synthesis of semiconductor nanowires by solution-phase and chemical vapor deposition (CVD) approaches to produce single crystal nanowires, radial/axial heterostructured nanowires, and complex architectures consisting of Si/Ge, III-V and other compound semiconductor materials. Future directions include using microfluidic methods to have dynamic control and *in situ* monitoring during Flow-Solution-Liquid-Solid growth.

- A wide variety of unique metamaterials and plasmonic nanomaterials can be fabricated on passive dielectric substrates or active semiconductor heterostructure substrates to create artificial atoms with tunable physical properties beyond those possible with ordinary materials. We will continue to create new material combinations and structures to exploit the reduced dimensional and interfacial physics in these material systems.

- CINT's Semiconductor Molecular Beam Epitaxy (MBE) is in demand worldwide to grow high-purity, ultra-high mobility As-based III-V compound semiconductor structures with atomic monolayer precision for fundamental studies of 1-D and 2-D nanomaterials. Our future plan includes extending our MBE capabilities to group IV materials to provide users with a new family of 2-D layered materials.

- Epitaxial and nano-composite films with specific electrical, optical, magnetic, thermal, and/or superconducting properties are grown by Pulsed Laser Deposition (PLD), Polymer Assisted Deposition and Laser MBE. Upgrades in progress will enable us to grow *epitaxial nanocomposite films* incorporating nanoparticles of controlled particle sizes and densities at desired locations.

- Our newest capability under development with users is Atomic-Precision Lithography as illustrated in Figure 12, which involves the placement of phosphorus donor atoms into silicon by hydrogen resist lithography in combination with scanning tunneling microscopy. *CINT is one of only two institutions in the world with this capability.*

Figure 12. Atomic Precision Lithography

The **CINT Integration Laboratory** is a class 1000 cleanroom with a comprehensive suite of micro/nanoscale tools including Atomic Layer Deposition (ALD), Low Pressure CVD, Physical Vapor Deposition, Electron Beam and Photo Lithography, Focused Ion Beam. Future capability enhancements include the creation of a soft lithography capability to enable users to fabricate and integrate soft/hard nano/microstructures, expansion of deposition/etching tools to meet user demand, addition of noble metal ALD, and replacement of legacy tools with current generation commercial tools.

4.3 Characterization

CINT current characterization capabilities include and extensive array of differentiating techniques to determine structural coordinates with atomic resolution, chemical composition, and temporal behavior for individual nanostructures to complex integrated environments. Our future emphasis will be to develop methods to extract such information from increasingly complex hierarchical materials with nanoscale to mesoscale complexity. Development of advanced probes plays a critical role in high-impact nanoscience discoveries and innovation of next generation technologies.

- The Super Resolution Microscope is an R&D100 award-winning microscope (shown in Figure 13) based upon single molecule detection that can be used to dynamically image nanomaterials in biological environments. Planned enhancements in temporal resolution and dynamic range will keep this capability at the state-of-the-art for single nanoelement and single molecule imaging and spectroscopy.

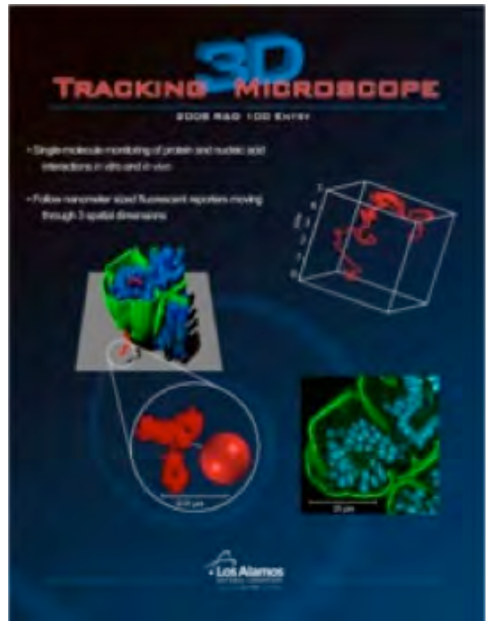


Figure 13. R&D 100 award winning 3D Tracking Microscope.

- Transmission Electron Microscopy capabilities at CINT offer an array of *in situ* techniques for correlating dynamic structural information with associated electrical, mechanical or compositional changes. CINT Discovery PlatformsTM are routinely employed as *in situ* TEM sample holders to provide unprecedented fundamental information on liquid/solid interfacial reactions, individual nanowires and related structures. CINT future plans for TEM include: significantly expanding our capacity to meet the consistent demand for instrument time by highly-ranked user proposals; adding aberration-corrected TEM to the user program to remain internationally competitive; offering a new suite of *in operando* capabilities as identified in the recent DOE workshop on the future of electron scattering; and developing the expertise/techniques for soft/composite nanomaterials microscopy needed by the integration challenges in section 2.

- Ultrafast Optical Spectroscopy offers unmatched ability to differentiate the dynamics of spin, charge, and lattice, and coupling between them in time and spectral domains because these interactions have different energies and occur at different characteristic timescales. Moreover, the available femtosecond pulse duration enables characterization of the dynamic response of a wide range of materials. CINT has a full range of time-integrated and time-resolved optical tools, covering the terahertz (THz) through the x-ray frequencies, to investigate the fundamental mechanisms of a wide range of nanostructured materials. Future enhancement to this capability are planned that will expand the available wavelengths, pulse energies and temporal resolution.

- CINT is establishing a new, comprehensive optomechanics capability with the ability to study phonon-mediated optical squeezing, single-photon optomechanics, and related phenomena in individual nanostructures.

- The quantum transport capability is includes multiple instruments configured for measuring low temperature electrical transport in semiconductor devices. We have demonstrated single shot electron spin measurements and rapid pulsing of the semiconductor nanostructure energy levels using these advanced techniques.

- CINT is currently the only NSRC with a dedicated nanomechanics capability, which includes ex-situ nanoindentation and electrical contact resistance measurements, integrated Atomic Force Microscopy, and oscillatory load cells. These are complimented by *in situ* straining stages for the Scanning Electron Microscope (SEM).

- The CINT Nanomanipulator (shown in Figure 14) is a custom two-probe device inside a scanning electron microscope for *in situ* quantitative nanostructure electrical and mechanical characterization.

Figure 14. CINT's custom built nanomanipulator.

- A recent addition is the Holographic optical trapping and force measurement system, comprised of a modular optical trapping fluorescence microscope that enables the non-contact 3-dimensional manipulation of trapped objects and a force measurement module capable of measuring pico-Newton interaction forces. The technique allowing one to study the unfolding of supramolecular structures, molecular motor action, and surface adhesion forces of biological cells.

- CINT offers users a combined atomic force and time-correlated single-photon (TCSPC) fluorescence imaging capability. This has proved invaluable for the study of the photophysics of small quantum dot clusters as well as the direct determination of dark/bright fractions of quantum dots.

- Broadband terahertz time-domain spectroscopy (THz-TDS) provides simultaneous amplitude and phase information, and is a powerful tool for the characterization of materials and devices including semiconductors, complex metal oxides, multiferroics, metamaterials.

- The low energy electron microscope (LEEM) is a unique and versatile surface microscope that can be used to view dynamic processes on surfaces in real time with a spatial resolution of 7-8 nm and a depth resolution of one atomic layer. Photoelectron microscopy and dynamic experiments will be enabled by the addition of pulsed laser light sources.

The CINT Near-IR microscopy capability is built around an inverted microscope system that offers both confocal (diffraction-limited) excitation for rastor-imaging, and wide-area excitation for direct 2-D imaging, allows simultaneous imaging with real-time access of differing spectral regions.

4.4 Theory, Simulation and Modeling

The unique properties of nanostructured materials cannot be fully exploited without a predictive understanding of the underlying phenomena. This requires a spectrum of theory/simulation techniques developed and optimized not only for the nanomaterial component itself but also for its interactions with surrounding components and materials. Some of the specialized techniques being used, under development and planned include:

- Theory of correlated systems and exact dynamics simulations are paired with exquisitely detailed data obtained from our ultrafast spectroscopy experiments to elucidate the physics of carrier transport in individual, ensemble and composite nanomaterials.

- The Exciton Scattering Model as illustrated in Figure 15 is a unique CINT capability that enables simulations of excitonic behavior in much larger and more complex structures compared to traditional approaches.

- Our Non-adiabatic Excited State Dynamics capability can handle larger systems than fully ab initio approaches while maintaining a realistic treatment of excitonic physics and the non-adiabatic processes.

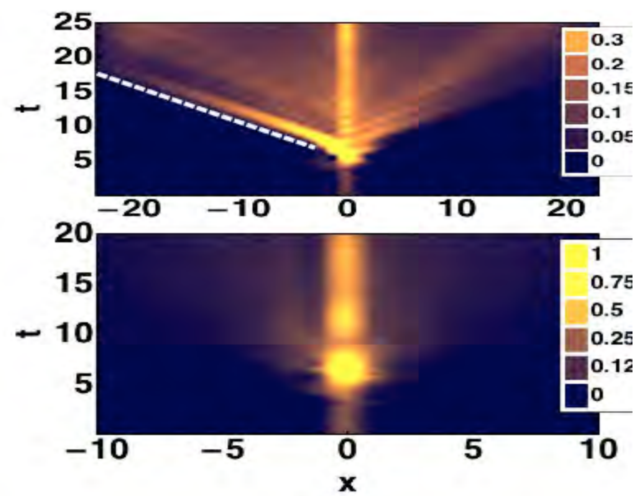


Figure 15. A polaron quasiparticle (an electron dressed by fully quantum phonons) in a nanowire is excited by an ultrafast optical pulse.

- The Exact-Diagonalization approach to quantum-correlated dynamics was developed at CINT and provides an essentially exact solution to problems, where previously only approximate solutions were available.

- In response to the rapidly increasing interest in soft, biological and composite nanomaterials, CINT continues to develop methods to model soft/hard material interfaces for systems such as polymer nanocomposites, biomolecule/materials and nanoparticle self-assembly using classical density functional theory, self-consistent field theory, molecular dynamics simulations, and Monte Carlo simulations.

- The nanoscale structure and properties of interfaces and atomic-scale defects can be elucidated by first-principles Kohn-Sham density functional theory, time-dependent density functional theory, the cluster expansion approach, and kinetic/statistical Monte Carlo methods. Future efforts will focus on quantum many-body first-principles simulations of hybrid structures, which have the potential to address strong electronic correlation effects.

- Our Time Dependent Density Functional Theory (TDDFT) approach shows the potential of being the first method to understand electron-ion heat exchange and electronic heat transport in nanostructures.

5.0 Engaging the National/International Scientific Community

Realization of our vision of nanoscience integration will continue to require the active engagement of our user community through a variety of mechanisms that both promote the essential practices of integrating nanomaterials and serve to build robust communities around key integrations challenges that by their very breadth and complexity transcend individual project/investigator efforts.

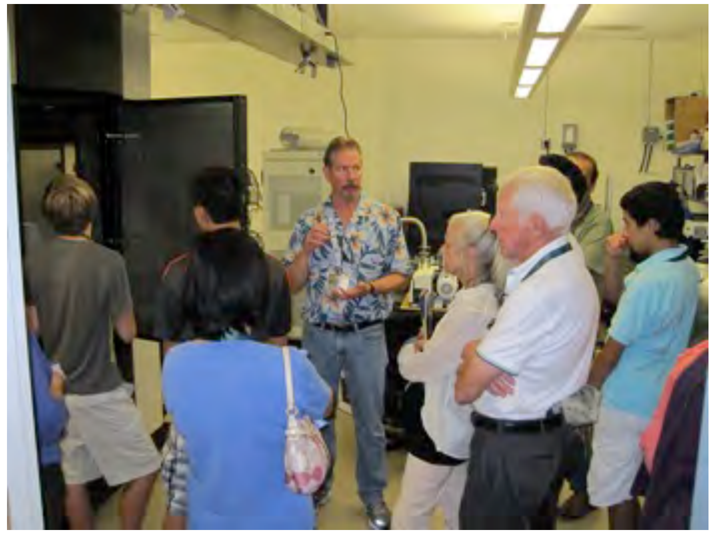
One of CINT's main goals is to attract research leaders in diverse institutions, early career scientists, and innovators in nanotechnology companies to create an expanded user community. To achieve this, it is necessary to target outreach activities that would increase awareness of our existing portfolio and capabilities within this identified group. We must have continued presence in high-profile journals, organizing symposia at national meetings and targeted workshops on nanomaterials integration challenges, hosting high-profile seminar series, and demonstrating the full suite of CINT capabilities and how users can utilize our expertise within all aspects of integration. We plan to take advantage of the NSRC Portal as one way for users to identify CINT capabilities and expertise.

CINT's Integrated Focus Activities are already attracting a collection of experts and young scientists dedicated to solving challenges in metamaterials, nanowires, and programmable membranes. Through these networks, we have begun, and will continue to develop collaborative communities of scientists, sharing ideas, and working together to speed up development of the technological innovations that will come from solving these challenges.

To best take advantage of the user facility model, we are currently working on the development of partner user agreements. These partner users would guarantee access in return for an investment in CINT. While investment in an instrument is most common, other forms of investment from a partner user could include intellectual investment or expertise shared with CINT staff and other users. Partner user agreements will assist us in remaining in the forefront of nanoscience, through the development of new, targeted capabilities.

The success of nanoscience integration will be in the ability to incorporate the basic science techniques within an engineering application. CINT is in a unique position to bring together the science and engineering expertise of LANL and SNL to expedite the development of nanomaterials integration. Our users and staff are already working with engineers at SNL to design and develop the Discovery Platforms. This is a partnership that will continue and broaden as nanoassemblies become included in chips and other electronic devices.

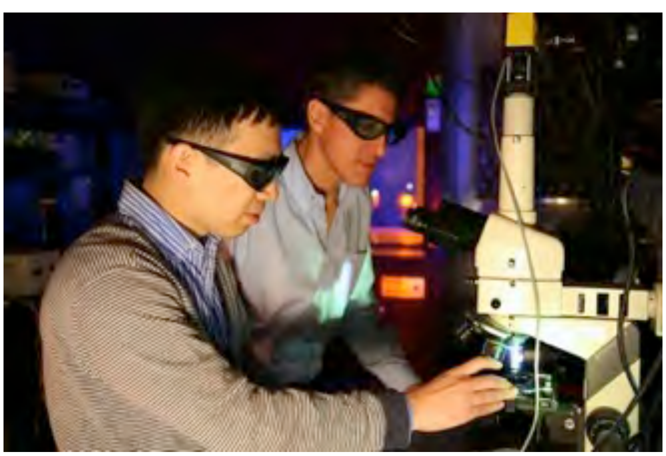
6.0 Operational Excellence



CINT has increasingly developed an identity that transcends Laboratory boundaries, striving for operational "best-in-class" performance at the Center. Efficiency is at the forefront of our business operations focus. We have adopted and embedded standard project management principles and methodologies that continue to be applied throughout the Center to ensure operational efficiencies and impactful cost savings.

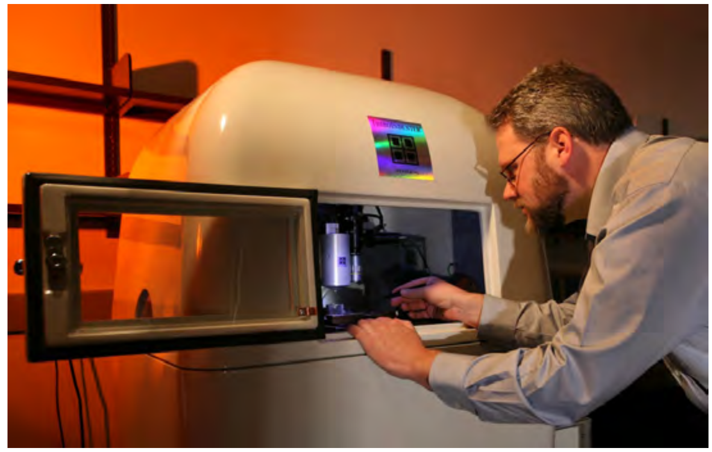
The realization and implementation of the online User Program Management System will allow us to improve business intelligence operations throughout the Center. This system allows for creating workplace efficiency by leveraging digital technology to decrease the amount of manual hours lost on easily automated tasks and enabling the support of an increased number of users. The tool will increase data accuracy and maintain a shared repository that will provide historical, current and predictive views. This data will allow CINT to track trends in the user program to allow for better decision-making in capability development and stay abreast of increasing science focus areas within our user communities.

With the pool of dedicated scientists available through our Users Executive Committee, Science Advisory Committee and users in general, CINT is well poised to look for trends in nanomaterials integration across the nation and the world. Between these personal interactions, and the ability to see trends across the user program, CINT will be poised to respond to the needs of the nanoscience community. This information will help to fill gaps in available capabilities, both through the development of specialized instrumentation and in the collective expertise of CINT staff and user community. Strategic hires of staff and postdoctoral researchers will be based around the needs of the community and addressing integration grand challenges.



As with any business operation, CINT is constantly benchmarking best practices for improving on processes and procedures. We have the opportunity to lead the complex in improving cross-laboratory processes, in particular with a goal of creating a training program that would be acknowledged at both Los Alamos and Sandia national laboratories.

7.0 Implementation

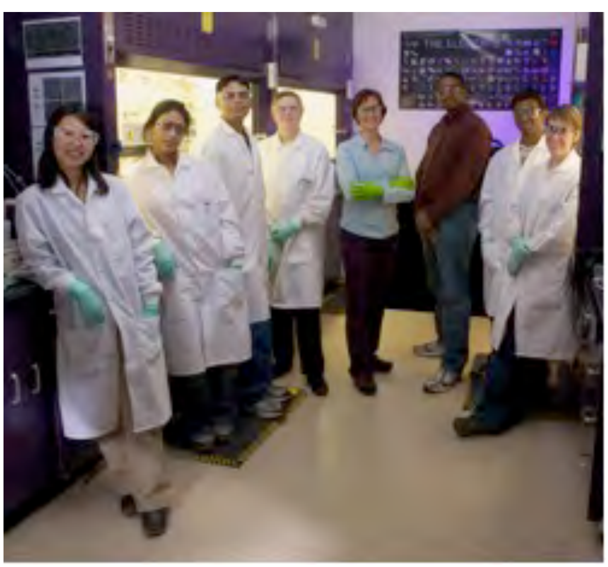


CINT 2020 presents a vision for potentially revolutionary new technologies that would be enabled by integrating nanostructured materials to exploit their size-dependent properties or emergent collective properties. Realization of this opportunity requires a sustained effort by researchers to tackle more complex nanosystems; however, the optimal methods to do so may not necessarily exist today or may not be available to researchers with extraordinary ideas and insights.

CINT's differentiating focus on nanomaterials integration and established operation as a DOE/SC user facility with a vibrant, growing user community, together position us to be a leader at this new frontier in nanoscience. Our six strategic objectives drive us towards the goal of being the national resource for *research expertise* and *advanced capabilities* to create, characterize, and understand nanostructured materials in increasingly complex integrated environments.

The strategy involves harnessing the intellectual leadership and scientific expertise of our staff and users (objectives 1 and 6) by adding CINT scientists and attracting international experts as CINT users. A second strategy complements the people in our community with the capabilities that we invent or optimize for integration research (objectives 2, 3 and 4), thereby ensuring that CINT is unsurpassed as an institution for our chosen areas of nanoscience. In an increasingly competitive world, CINT must also continuously focus its efforts and resources on the potentially most impactful research opportunities (objective 5). This will be done through organized CINT workshops, the CINT Annual User Meeting, joint-NSRC workshops at major national scientific conferences, consultation with the CINT Scientific Advisory Committee and the CINT Users Executive Committee.

The implementation of this Strategic Plan will be tracked and guided by more specific operational plans with annual milestones and actions toward each of the strategic objectives. Progress towards the milestones and refinement of directions will be reviewed semi-annually by the CINT leadership team.



When the National Nanotechnology Initiative was launched over a decade ago, the nation was at the dawn of the next technological revolution. Since then, amazing scientific discoveries have validated the promise that small is different. Just as integration transformed the transistor into the integrated circuit, now the scientific community is prepared to reveal even greater wonders by learning how to build a world of functional materials that can begin to rival the exquisite examples we see everyday in nature.