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Future Directions – CINT 2024

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Overview

- Scientific Mission Statement – “Nanoscale Integration”
- CINT’s Strategic plan (CINT 2024)
  - Planning process and purpose
  - Scientific opportunities in integrated nanotechnology: QIS, Hybrid- and Soft-Materials
  - Capabilities in development
- Machine learning (beyond CINT 2024)
- Users: Targeted outreach
- MIE proposal
- Staff: Self-evaluation
- Connections to hosts labs

CINT – Scientific Mission Statement

CINT's mission is to provide scientific understanding underlying nanoscale integration through the assembly of diverse materials across multiple length scales, with the ultimate goal to design and control new material properties and functionality.

Nanostructured materials gain value when integrated with other components

Integration of Nanomaterials

InP/CdSe type-II gQDs

- (a) Dip-Pen placement of QDs onto all-dielectric antennas
- (b) k-space image of photoluminescence from a single QD placed in the center of a metallic bullseye antenna w/o dielectric layer.
- (c) Same QD w. dielectric layer → directional single-photon source

We review and update the Strategic Plan every year (January).

Purpose:

- Lay out future scientific directions to strengthen for the 5-year time frame
- Inform our staffing and recapitalization decisions
- Align CINT with BES mission and strategic priorities

Characteristics:

- Well-defined and actionable
- Differentiate CINT from other NSRCs
- Integrate with the host labs' strategic plans

Informed by:

- Ideas are initiated by CINT scientists, users, and discussed with the SAC and UEC

CINT2024 emphasizes areas we want to strengthen

CINT's Strategy Embodies DOE and BES Goals

National Nanotechnology Initiative

Goal 1: Advance a world-class nanotechnology research and development program.

Goal 2: Foster the transfer of new technologies into products for commercial and public benefit.

Goal 3: Develop and sustain educational resources, a skilled workforce, and a dynamic infrastructure and toolset to advance nanotechnology.

Goal 4: Support responsible development of nanotechnology.

CINT's Strategy: be a Key Player in the NQI

NATIONAL
STR

National Science
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THE NATIONAL
NANOTECHNOLOGY
SUPPLEMENT
PRESIDENT'S

Basic Energy Sciences Roundtable

**Opportunities for Quantum Computing
in Chemical and Materials Sciences**

Basic Energy Sciences Roundtable

**Opportunities for Basic Research for
Next-Generation Quantum Systems**

One Hundred Fifteenth Congress of the United States of America

AT THE SECOND SESSION

*Begun and held at the City of Washington on Wednesday,
the third day of January, two thousand and eighteen*

An Act

To provide for a coordinated Federal program to accelerate quantum research and development for the economic and national security of the United States.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

SECTION 1. SHORT TITLE; TABLE OF CONTENTS.

(a) SHORT TITLE.—This Act may be cited as the “National Quantum Initiative Act”.

(b) TABLE OF CONTENTS.—The table of contents of this Act is as follows:

Three Major Nanoscience Opportunities Targeted by CINT

CINT is invested in strengthening the following three areas in the next 5 years:

- (1) Understanding the origins and controlling quantum phenomena in quantum materials systems;
- (2) Creating hybrid material interactions for the generation and manipulation of light particularly in the area of metamaterials;
- (3) Soft Nanomaterials Science: synthesis, assembly integration, characterization and theory;

(I) Understanding the Origins and Controlling Quantum Phenomena in Quantum Materials Systems

Expand and develop capabilities to support users in QIS:

- Provide a broad spectrum of ion sources for implantation
- Deterministic placement of color centers in host materials
- Scanning probe methods to fabricate optically active sites
- Characterization of individual defect sites

2 new projects
additional \$8M

QSNMR platform

Future projects:

- Using light to probe and control novel phenomena in quantum materials
- Understanding emergent and correlated phenomena in quantum materials
- Quantum-sensed Nuclear Magnetic Resonance (NMR) Discovery Platform™ for localized spin sensing

(a) FIB implantation of Si into diamond
(b) PL of hBN flakes from local defects

Deterministic Placement of Color Centers: Implantation and Chemical Functionalization

CINT user projects

Diamond NEMS cantilever.
(Inset) fluorescence from SiV— centers

Y.-I. Sohn, et al. *Nature Communications*, 2018

R.E. Evans, *Science*, 2018

Photon-mediated interactions between pairs of silicon vacancy centers embedded in a diamond nanocavity (Photonic crystal).

Chen-Yen Lai, *Nanoscale*, 2019

Understanding light emitters in quantum nanostructures

Optical absorption spectrum of anisotropic coupling systems with nanoparticle center.

Dip-pen nanolithography “Chemical Implanter”

F. Dawood, *Small* 2018

(2) Hybrid Material Interactions for Generation and Manipulation of Light (incl. Metamaterials)

- Materials and assemblies that generate and harvest electromagnetic energy
- Hybrid materials and structures that control electromagnetic energy (plasmonics and metamaterials)

Future projects:

- Active, multifunctional plasmonic and metamaterial interactions with switchable and highly tunable photon emission. (e.g. biexciton emission, metamaterials with dopant states, soft materials to modulate interaction between emitters, metamolecules)
- Driven quantum matter: Using light to probe and control novel phenomena in quantum materials
- Nonadiabatic excited-state molecular dynamics to model to the largest systems

Single photon sources

Controllable metamaterials

Hybrid Materials – Light Interactions

CINT user projects

The first demonstration of efficient cascaded energy transfer of the multiexciton states of “giant” nanocrystals into underlying silicon substrates

Tianle Guo, et al, *Nanoscale* 2017

Growing crystalline materials on 2D materials

J.Yoo et al., *Nanoscale*, 2018

Hybrid graphene metasurface, enables the control of reflection spectra when applying gate voltages

B. Zeng et al., *Light: Science & Applications* 2018

Photodetector: lateral Graphene p-n junctions via ion implantation

G.Wang, et al., *Nat. Comm.* 2018

(3) Soft Nanomaterials Science: Synthesis, Assembly, Integration, Characterization and Theory

- Enhanced molecular and nanoscale building blocks that directly assemble and integrate
- Approaches to assemble heterogeneous nanocomponents across multiple length scales and dimensionality

Future projects:

- Preparation of synthetic (e.g. polymers) and biomolecular nanomaterials (e.g. peptides and proteins) with self-assembly instructions – key characterization tool will be CryoEM
- Assemble nano-building blocks that form highly dynamic and far-from-equilibrium states (e.g. self-healing)
- Self-consistent field theory, Monte Carlo simulations and molecular dynamics package (LAMMPS)
- Molecular electronic structure database for machine learning

Microfluidic Discovery Platform™

Cryo-TEM images of coated mesoporous silica nanoparticles

Soft Nanomaterials Science

CINT user projects

Movement of a flexible magnetic composite is achieved with the interplay of photothermal effect and temperature-induced demagnetization by light

Working principles of the actuator

A magnetic elastomeric composite being actuated by green light and a permanent magnet

Meng Li, et al., *PNAS*, **2018**, 8119

nanoparticles grafted with two different immiscible polymers can form Janus phases in solution that are robust to fluctuations

no fluctuations

with fluctuations

Koski & Frischknecht, *ACS Nano*, **2018**, 1664

E-Waste upcycling & formation of metal nanoparticles via ultrasonification

Watt et al., *Small*, **2018**, 1703615

Top: Schematic of dynamic recruitment of kinesin nanomotors for the transport of microtubule filaments.

Bottom: Time-lapse images showing deposition of motors (green) during transport of a microtubule (red). Scale = 5 μm

A.T.C. Lam, et al., *Nano Letters*, **2018**, 1530

molecular-scale system that dynamically assembles and disassembles

Integrate Artificial Intelligence with Science Thrusts

Rationale:

Big Data in experiments & simulations

Nanophotonics

Deep Learning & Optimization

Waveguides, On-chip devices,
Metamaterials

Impact:

Tight coupling between thrusts
Training/job opportunities for postdocs, new
users, high quality publications

Quantum Materials

D-Wave

Quantum Machine Learning

Artificial Intelligence

Soft Materials

Function Learner Neural Network

Characterization & Nanomechanics

Deep Learning to model
microscopy data

CINT 2025 discussion

User Meeting in 2019:
Workshop and Focus Sessions on
machine learning (w. all NSRCs)

Nanomaterials Discovery Enabled by Machine Learning

DNA selects sizes and fluorescence colors of DNA-stabilized silver clusters through a poorly understood process. We combine high throughput experiments with machine learning to uncover the mechanisms selecting size/color.

Colors of silver clusters stabilized by training DNA sequences (grey) are compared to sequences designed to stabilize clusters with fluorescence < 580 nm (green) and > 660 nm (red).

Scientific Achievement

First design tool for fluorescent silver clusters with control over fluorescence color, by combining machine learning with large data sets.

Significance and Impact

Promising biosensors, exhibits the potential of machine learning and data mining to increase precision and efficiency of nanomaterials design.

Research Details

DNA-stabilized silver clusters were synthesized and characterized in high throughput to create the largest data library connecting DNA sequence to silver cluster fluorescence color.

Machine learning and bioinformatics were used to learn the DNA base patterns that select for silver cluster color/size.

New DNA sequences are designed by trained machine learning classifiers to stabilize silver clusters with fluorescence in certain desired color bands, and designs are experimentally verified.

S. M. Copp, A. Gorovits, S. M. Swasey, S. Gudibandi, P. Bogdanov, E. G. Gwinn **ACS Nano** 12, 8240 (2018).

Tools and Capabilities in Development

Capabilities

- (1)
  - Deterministic placement of color-centers
  - Quantum Sensed-NMR
- (2)
  - NEXMD: Non-adiabatic excited state molecular dynamics codes (modeling photophysics & chemistry in the presence of environment)
  - Expansion of single photon detection capabilities to the mid-IR
- (3)
  - Femtosecond mid-IR microscopy (extended wavelength response and dynamics of emerging metamaterials and for probing of phonon coupling)
  - THz Circular Dichroism Spectrometer
- (3)
  - CryoEM suite: SEM/FIB, TEM and vitrobot

NEXMD Code

Cryo-TEM

Major Item of Equipment (MIE) Proposal

Capabilities

Recapitalization proposal for the NSRC program

Strategic investment in emerging areas of nanoscience, designed to ensure continued U.S. leadership in the basic science underlying the most important materials advances of the upcoming decade

Task 1: Expanding the Limits of Nanofabrication

- Radical Lithography for Nanoscience
- Depositing Heterogeneous Materials with High Precision
- Sculpting Next-Generation Nanomaterials

Task 2: Accelerating Nanoscale Materials Discovery and Design

- Autonomous Synthesis Across Scales
- Transformative Research Capabilities for Imaging and In-situ Characterization
- Computing and Data for Integrated Instruments

Task 3: Decoding Nanoscale Dynamics and Heterogeneity

- Charge, Spin, & Structural Dynamics of Materials
- Atom-scale Understanding of Environment Effects & Chemical Heterogeneity
- Measuring the Dynamics of Disorder, Distortions, & Transport at the Nanoscale

Received Critical Decision 0 – Mission Need Established

Outreach and Connection to the Scientific Community

Users

Targeting new external users – joined forces with NSCRs:

- EFRCs, early career awardees, and other high-profile DOE programs to directly couple to DOE's broader mission
- Early career academics
- NSRCs joint MRS booth; effectiveness assessment led by CINT
- NSRC portal (hosted by CINT)
- Strengthen partnerships with other NSRCs (user meeting participation, staff seminars)

Self-Assessment: “State of CINT” a Look Inside

Staff

Approach:

- Conducted a grass roots assessment of how the CINT community feels the center is operating and performing
- Solicited community ideas and opportunities for improvement of operations

(*conducted by external consultant – D. Morris)

“CINT’s physical”

Outcome:

- Improved communication and transparency desired
- State of science and health of the user program deemed “good” or “very good”
- Strong sense of unity
- Positive feedback on strategic planning process

Actions:

- All-hands meetings restructured
- Group meetings with additional presenters
- Regular group updates via monthly email

CINT science underpins SNL and LANL missions

Host Labs

LANL

Strategic Objectives	Excellence in Nuclear Security	Excellence in Mission-Focused STE	Excellence in Mission Operations	Excellence in Community Relations
Critical Outcomes	Design, produce, and certify current and future nuclear weapons and reduce global nuclear threats	Deliver scientific discovery and technical breakthroughs that support DOE & NNSA missions	Execute sustained operations that are reliable and responsive to mission needs	Sustain and enhance LANL's partnership with the community across the Northern New Mexico region
Major Initiatives	- Execute LANL's manufacturing mission to deliver 30 plutonium pits per year - Transform nuclear weapons warhead and production - Anticipate the global security environment and develop and demonstrate revolutionary tools to detect, deter, and respond	- Refresh and refine the LANL capability pillar framework - Advance accelerator science, engineering, and technology to enable ECSE to DMMSC and related capabilities - Advance the frontiers of computing to exascale and beyond - Assert leadership in the national quantum initiative - Develop and implement an integrated nuclear energy and materials initiative	- Achieve culture change with an emphasis on organizational learning - Improve integrated planning across priority mission activities and infrastructure - Address critical issues related to NMC&A, nuclear safety, criticality safety, and waste - Implement systematic process improvement to drive increased rigor and efficiency in work execution - Enhance quality of work life, workforce planning, and training and development	- Institute a personal commitment to community service by LANL leadership - Engage in mission-centered workforce and pipeline development - Enhance small business participation in executing LANL scope across all directions - Implement a Community Commitment Plan to provide educational support, economic development, and philanthropic support to the surrounding community

ADVANCED SCIENCE & TECHNOLOGY

Integrates multidisciplinary efforts to advance the science of the possible for Sandia's missions

WEAPONS SCIENCE & TECHNOLOGY

Provides Sandia with foundational science and engineering capabilities to ensure the nation's nuclear stockpile is safe, secure, and effective

OFFICE OF SCIENCE

Leads creative, hypothesis-driven inquiry in fundamental science to promote national security and international scientific leadership

CHIEF RESEARCH OFFICER

Governs and leads research strategy and stewardship of capabilities at Sandia, including the Laboratory Directed Research and Development program. Responsible for leadership of technology transfer and Sandia's partnerships with universities, industry, and the state of New Mexico.

Leadership in NQI

AREAS OF LEADERSHIP						
Complex Functional Materials	Material Resilience in Harsh Service Conditions	Manufacturing Science	Actinides & Correlated Electron Materials	Integrated Nano-materials	Energetic Materials	Materials Dynamics

Key Message – Present and Future

- High scientific productivity and impact in all thrusts
- A productive and satisfied user community
- Significant capabilities leveraged at both host institutions
- Effective team providing efficient and safe operations of the CINT facilities

How did we get here:
strategy, staff, users, capabilities,
leveraging host labs

Feedback Welcome

- We are looking forward to your recommendations!
- We are grateful for the feedback from the last review.
- We took the feedback seriously and have developed actions to address it.
- The reviewers' feedback helped us improve and grow.

Thank you!

BACK UP

MIE – CINT Recap List

	Theme 1		Theme 2		Theme 3	
NSRC	Nanofabrication at the Limits	Est. cost (\$M)	Accelerated Nanoscale Material Discovery and Design	(\$M)	Decoding Nanoscale Dynamics and Heterogeneity	(\$M)
CINT	MBE - upgrade	\$1.5	Dynamic SIMS	\$3.0	ARPES	\$1.5
	Ion beam deposition	\$1.0	Multiprobe AFM system	\$0.8	Time resolved cathodoluminescence and current mapping	\$2.0
	eBeam lithography	\$3.0	Electrohydro-dynamic printing (EHD) / Softfab lab (Millie / Bachand / Jinkyong)	\$1.7	Light sheet microscope	\$1.0
	Proton Beam Etching	\$3.0				
	Silicon deep etcher					
	SiDRIE	\$0.8				
	RIBE/ Atomic Layer Etching	\$0.8				
\$20.0	Theme 1 Subtotal	\$10.0	Theme Subtotal	\$5.5	Theme 3 Subtotal	\$4.5