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BES Triennial Review

Center for Integrated Nanotechnologies (CINT)

Andreas Roelofs – Director

Wahid Hermina – Co-Director (acting)

May 14-16, 2019



Sandia
National
Laboratories



Los Alamos
NATIONAL LABORATORY
EST. 1943

- LAUR

Key Message

- 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



CINT Overview Topics

- CINT's vision, mission, and structure
- Host labs capabilities and connections
- Environment, Safety and Health
- Differentiating capabilities in nanoscience
- Growth in user community, productivity, and scientific impact
- Brief future opportunities and outlook
- Response to BES recommendations of 2016 review



CINT's Vision: "One scientific community focused on nanoscience integration"

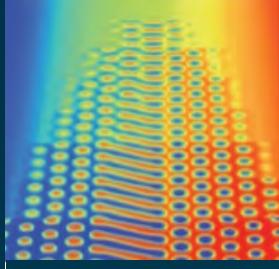


The DOE/SC nanoscience centers are different from traditional user facilities

- Defined by a scientific field, not specific instrumentation.
- NSRC staff support user projects and conduct original research.
- Capabilities involve hardware plus research expertise.



NSRC: Nanoscale Science Research Center



User Mission

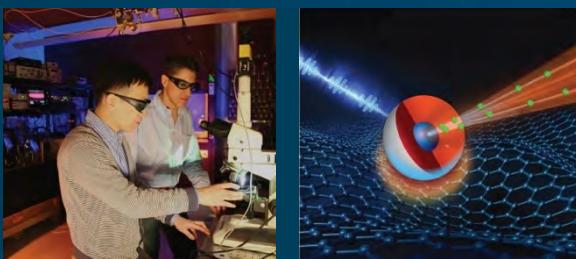
Provide users with world-leading scientific expertise and capabilities

Scientific Mission

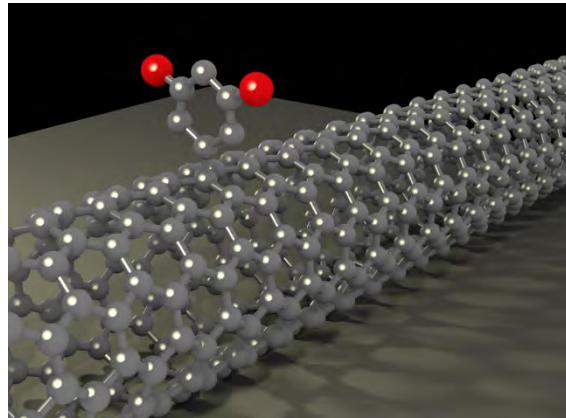
Provide scientific understanding underlying nanoscale integration through the assembly of diverse materials across multiple length scales, with the ultimate goal to design and control new material properties and functionality

Scientific Thrusts

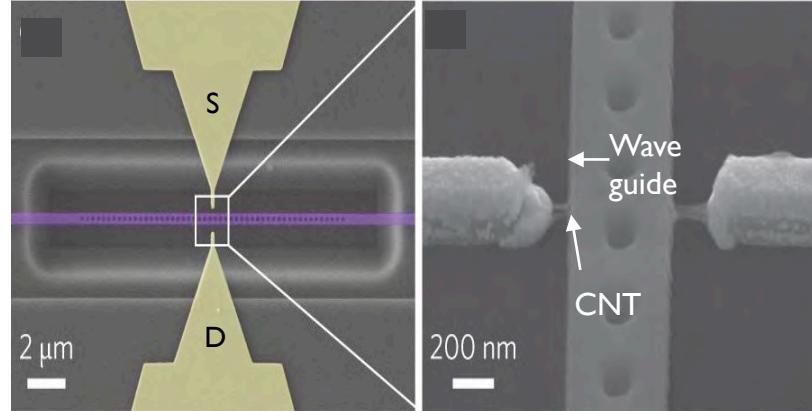
- Quantum Materials Systems
- In-situ Characterization and Nano-Mechanics
- Soft, Bio and Composite Nanomaterials
- Nanophotonics and Optical Nanomaterials



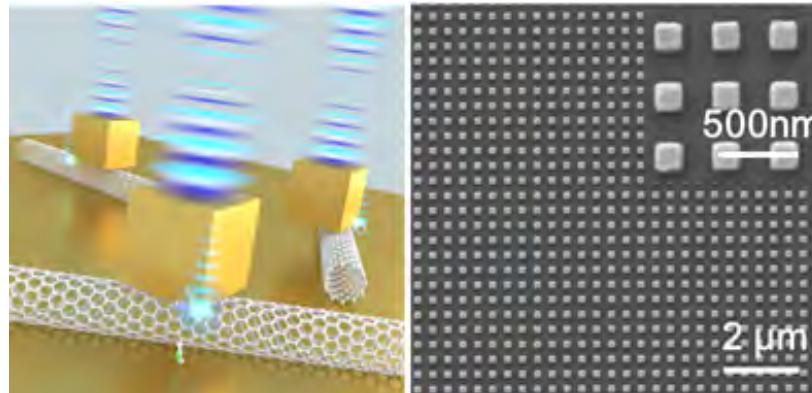
Concept of Integrated Nanotechnologies



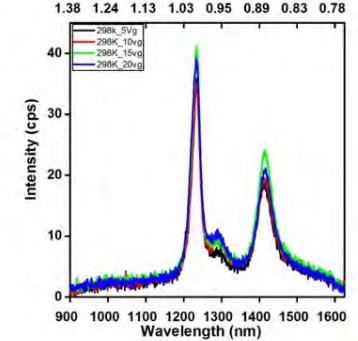
Functionalized Nanotube



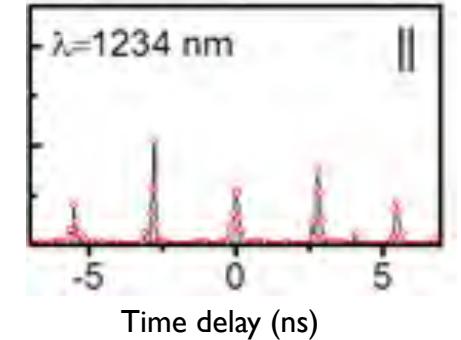
Nanotube Field Effect Transistors



Coupled to Plasmonic Cavities



Future: Electrically Driven Single photon emission



Indistinguishable single photon emission

CINT is One Community Focused on Nanoscience



Core Facility (SNL)



Gateway Facility (LANL)



CINT Operations:

- Two Facilities (total 130,000 gsf)
- 56 scientists & technologists
- 10 CINT post-docs & students
- \$22.5M annual budget
- Peer-review proposal process
- No-fee for pre-competitive research
- Full cost recovery for proprietary research



Office of
Science



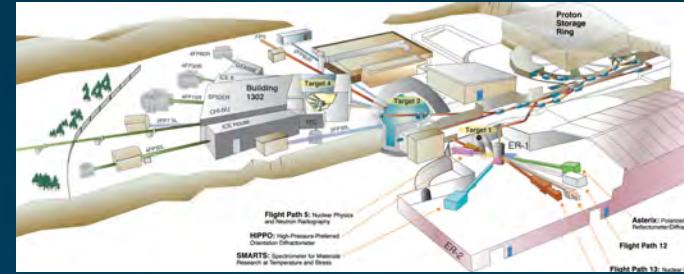
CINT Provides User Access to Significant Capabilities at both Host Institutions



Microsystems Engineering and Science Applications (MESA) Complex (SNL)



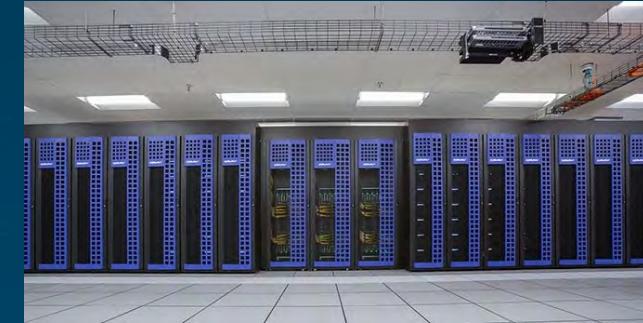
Ion Beam Labs (SNL and LANL)



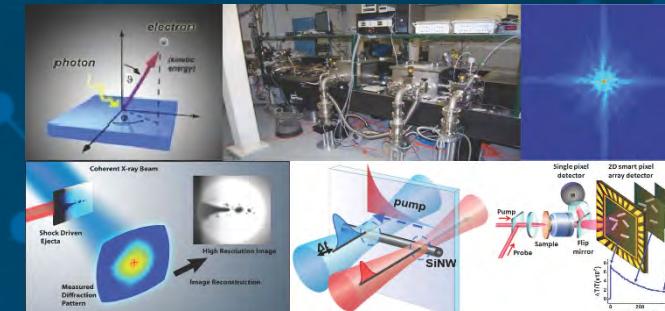
Los Alamos Neutron Science Center (LANSCE) (LANL)



National High Magnetic Field Laboratory (LANL)



High Performance Computing (SNL and LANL)



Laboratory for Ultrafast Materials & Optical Science (LUMOS) (LANL)

Integrated Safety Management (ISM)

Integrated Work Documents / Work planning and controls / Hazard analysis

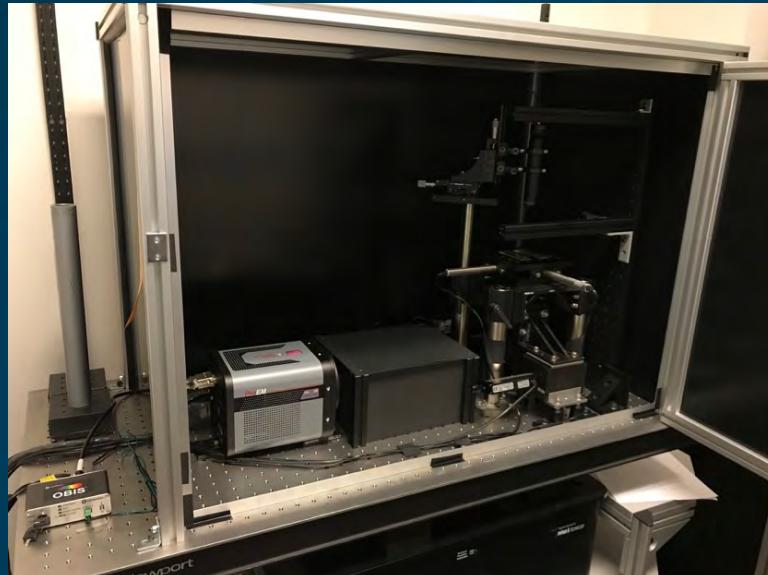
Reviewed by subject matter experts: Industrial Hygienists, Laser Safety Officers, Electrical Safety Officers and Pressure Safety Officers, & Chemical Safety Officers

- Exposure Assessments
- Medical Surveillance Programs
- Safety Training
- Waste Management
 - includes pollution prevention, waste minimization

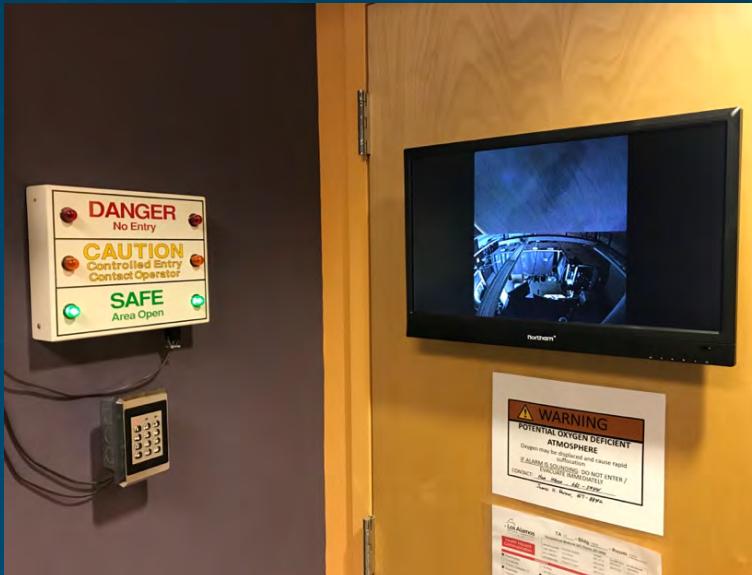


CINT is committed to safety and security

- Facility access is managed globally and at the individual lab level
- Use engineering controls where possible



Engineering control

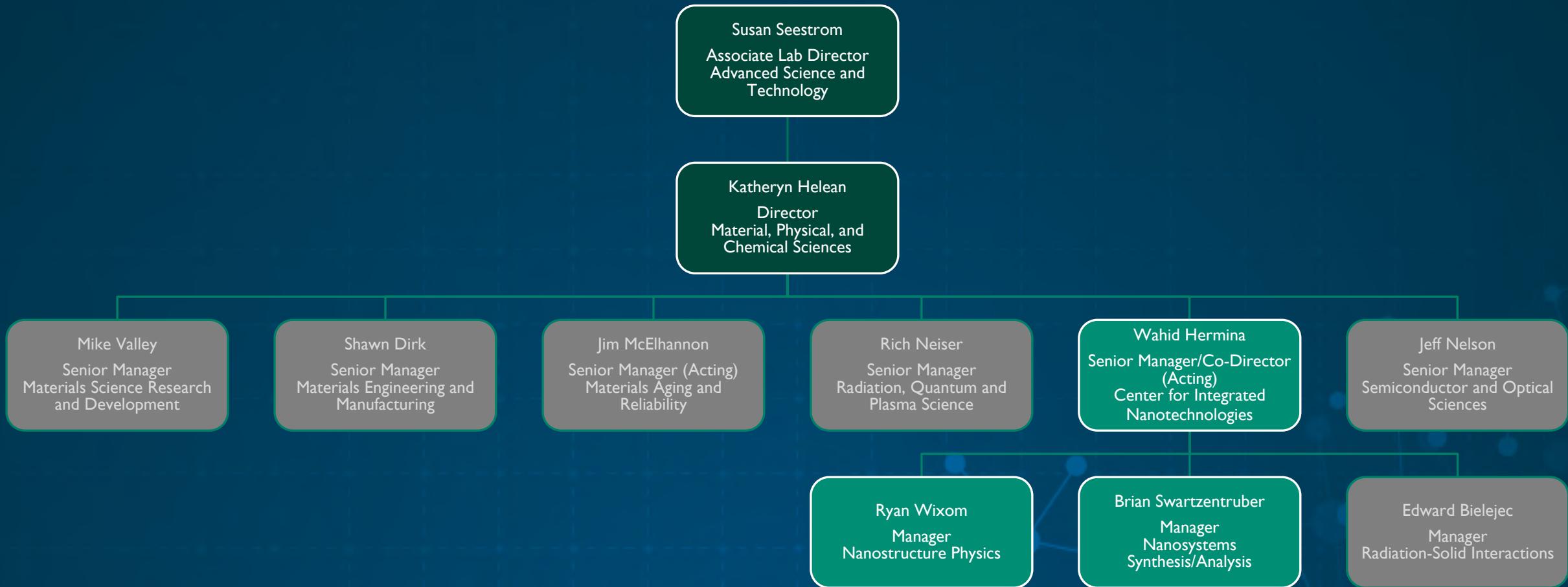


Best practice: virtual windows

LANL Organizational Chart



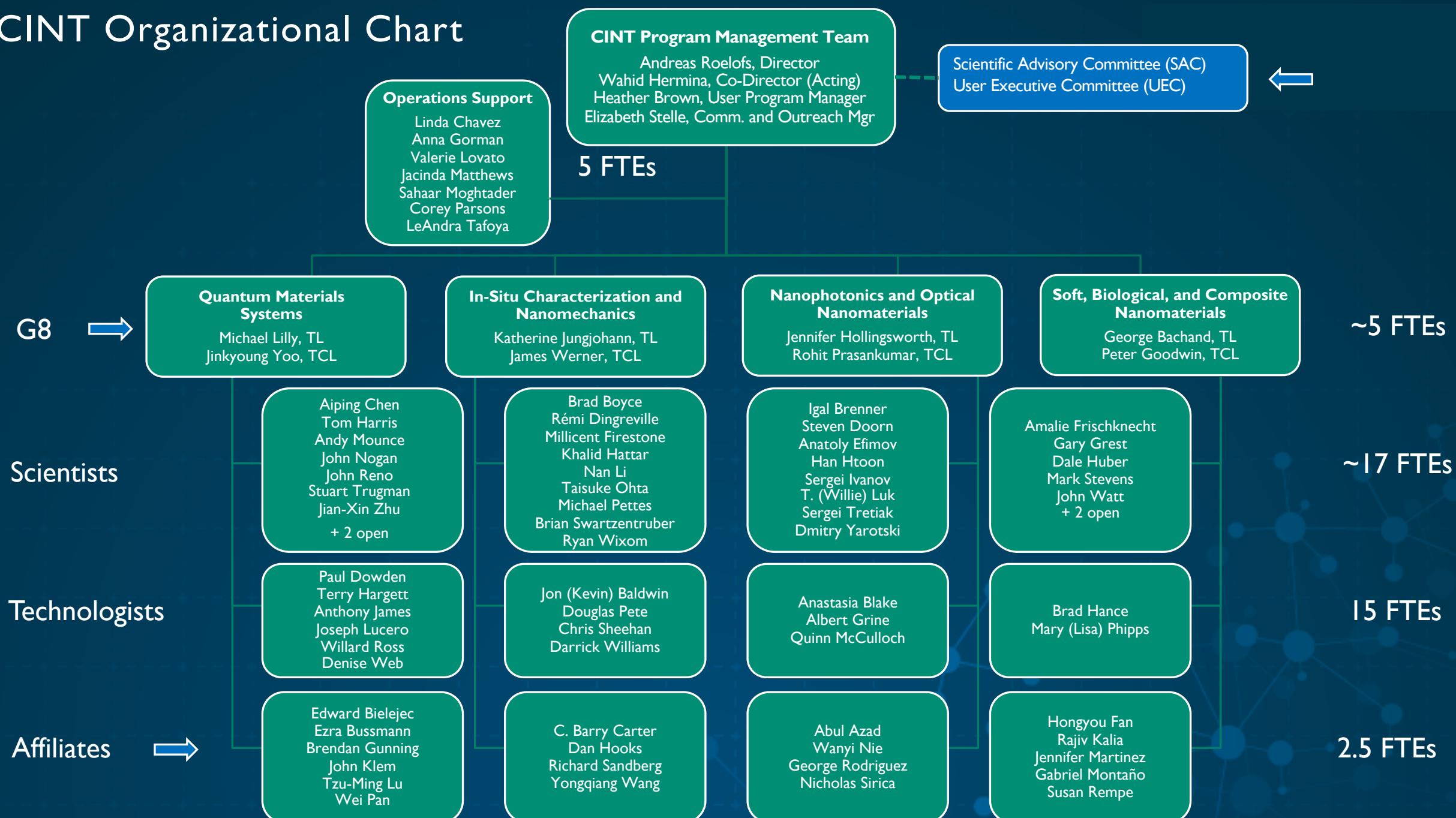
Sandia Organizational Chart



CINT High-level Organizational Chart



CINT Organizational Chart



Science Advisory Committee (“SAC”)

Rec #2 refresh SAC



Barbara Baird
Cornell University



Shef Baker
Cornell University



Dimitri Basov
Columbia University



Steve Brueck
University of New Mexico



Juan de Pablo
University of Chicago



Judith Driscoll
University of Cambridge



Rachel Goldman
University of Michigan



Mark Hampden-Smith
Saint-Gobain Innovative Materials



Jim Hannon
IBM /
Thomas J. Watson Res. Center



Don Lucca
(UEC Chair)
Oklahoma State University



Willie Padilla
Duke University



Andy Shreve
University of New Mexico



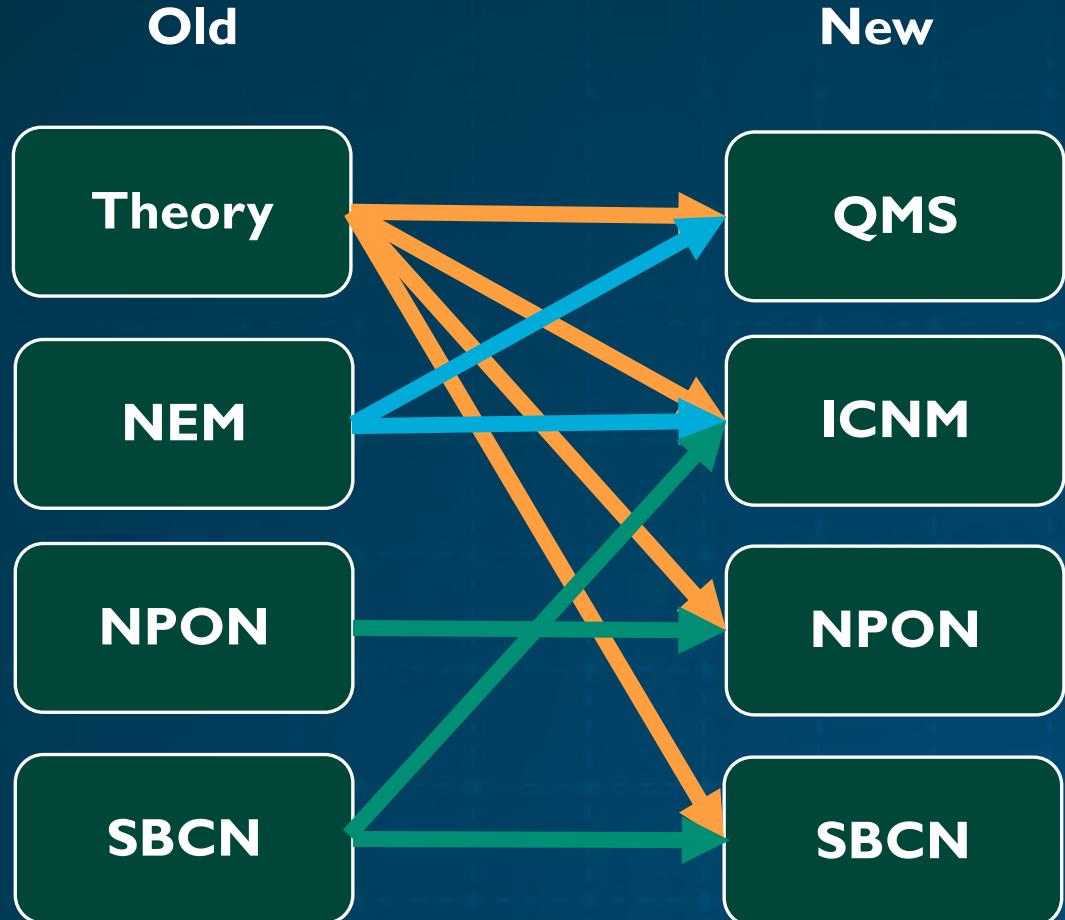
Ting Xu
University of California, Berkeley

- New Chair: Rachel Goldman
- 4 new members
 - Shef Baker, Cornell University
 - Judith Driscoll, University of Cambridge
 - Rachel Goldman
 - Jim Hannon, IBM
- Julia Fulghum, former Chair, rotated off after serving for 5 years.
- UEC Chair joined SAC

Heather introduces UEC / PRC

Restructuring of Thrusts (Feb-2018)

Rec #3, 7 publication goal, theory integration



- Enable growth
- Take advantage of synergy Exp. and Theory
- Highlight scientific strength to users

NPON: Nanophotonics and Optical Nanomaterials
SBCN: Soft, Bio and Composite Nanomaterials
ICNM: In situ Characterization and Nanomechanics
QMS: Quantum Materials Systems

CINT Science Leadership Team (“G8”)



Quantum Materials Systems



Mike Lilly

Nanophotonics and Optical Nanomaterials



Jen Hollingsworth

Soft, Biological, and Composite Nanomaterials



George Bachand

In-situ Characterization and Nanomechanics



Katie Jungjohann

Thrust Leaders



Jinkyung Yoo

Thrust Co-Leaders



Rohit Prasankumar



Peter Goodwin



Jim Werner

Gary Grest & Jian-Xin Zhu (Theory representatives)

Affiliate Scientists

Formalized CINT affiliate scientist expectations:

1. Is responsible for the operation of an affiliated CINT capability; and
2. Is expected to maintain a productive user base of ~5-10 users (for 0.25 FTE only for user science)*, that are publishing at a rate consistent with the expectations of the Office of Science.
3. Compliment a CINT thrust and participate in thrust and center level activities, (e.g., user recruitment, annual user meeting, triennial review.)
4. Is to contribute to the research lead by our CINT Scientists through collaboration on a project that he/she is leading and that will be reported as internal CINT science;
5. Affiliate positions are reviewed and renewed annually based on a report on their activities and accomplishments.

Affiliates allow users access to host labs capabilities

Growth and Scientific Impact 2016-2018



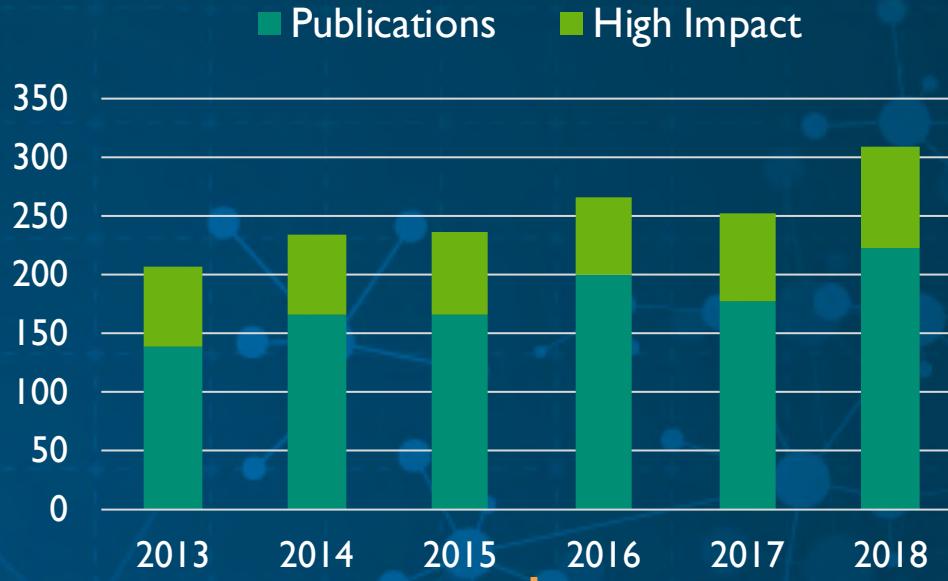
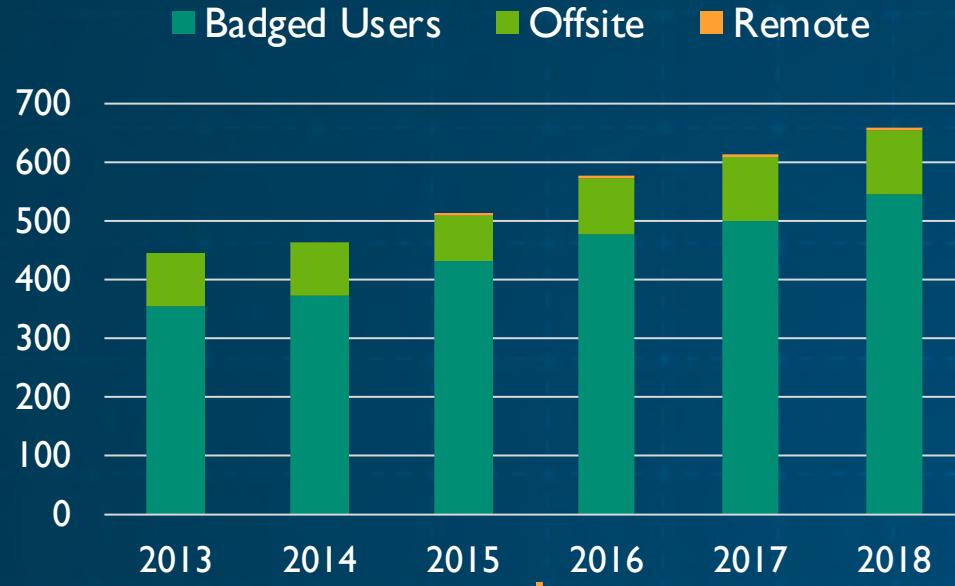
Rec #3 publication goal

973 user proposals (40% increase over previous review period), 773 accepted.

1847 total users (17% increase). Of these, 698 (38%) are first time users from 230 institutions in 27 countries.

828 journal articles (19% increase)
227 of those published in NSRC High Impact (10% increase)

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





We review and update the Strategic Plan annually (January)

Purpose:

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

Strategic goals:

- (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: synthesis, assembly integration, characterization and theory

CINT2024 emphasizes areas we want to strengthen

Recapitalization

Rec #4 10% Recapitalization

- High-speed single electron camera for in-situ TEM
- Coherent Inc.: Laser amplifier system
- Superconducting nanowire detector
- Gatan Ion Mill
- 9T Superconducting Magnet System for Microscopy Cryostat
- Ti:Sapphire regenerative amplifier laser system
- InGaAs Camera System
- Agilent Optical Emission Spectrometer
- FEI TITAN:Aberration corr.environmental TEM (**Host lab**)
- Cryostat with 5 optical ports and nano-positioning system
- Quantum Design: 3 Tesla Cryogen free PPMS
- Laser Scanning Microscope
- Hitachi: FlexSEM 1000, Cabinet Scanning Electron Microscope
- U9820A Keysight Nano Indenter G200
- Q800 Dynamic Mechanical Analyzer
- MIRcat-QT 2200 Laser System

Capabilities



- TECMAG INC: Nuclear Magnetic Resonance research system
- DPSS Laser System
- SHI Cryogenics Cryocooler
- Princeton Instruments NIRvana: NRL-640 InGaAs camera system
- StarShape 250 watt CO₂ Laser
- Metalorganic Chemical Vapor Deposition (MOCVD) System
- Plasma FIB (**Host Lab**)
- CryoEM (TEM/FIB)



\$50-90M MIE proposal (Recap of NSRCs) CD-0 approval

CINT's Recapitalization Principles

NSRC wide Recap goals:

Goal 1 – Establish new and unique capabilities for the future of Nanoscience

Goal 2 – Advance existing capabilities to maintain scientific leadership

Goal 3 – Uniqueness in the scientific communities and across NSRCs

Principles to build or acquire capability:

- 1) High user interest
- 2) Staff expertise, push and availability
- 3) Operational cost considered
- 4) Space

 **Center for Integrated Nanotechnologies**
Jointly Operated By:
Los Alamos National Laboratory
Sandia National Laboratories

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Cryo Electron Microscopy Suite for Low Dose Imaging of Soft Materials
Despite the tremendous work using Cryo EM to study biological materials, there are still significant new opportunities in the application of Cryo EM to study electron sensitive materials. We propose a unique and flexible system for minimizing electron dose in the imaging of soft materials and their interfaces to provide our user community with an optimized system for these sensitive materials.

The Cryo EM Suite contains 3 tools designed to image soft materials with an absolute minimum of beam damage. The suite includes a Vitrobot for optimized vitrification of samples and a CryoFIB for thinning and sectioning of vitrified samples. Finally, imaging occurs on the Talos L120C CryoTEM with a speed enhanced camera and a low-dose exposure technique utilizing a beam blanker. The combination of a low acceleration voltage TEM with low dose imaging and a complete set of cryo preparation tools will provide optimum soft matter imaging. This suite is unique among the NSRCs, and has been optimized contrast for imaging sensitive materials while minimizing beam damage.

 **Vitrobot**

 **Aquila CryoFIB**

 **Talos L120C TEM**

Impact to the User Program
More than 40 current users could benefit from an optimized soft materials imaging suite, and at steady state the suite is expected to add about 50 users per year. The specific research that would be enabled is widely varied, but several areas are described below.

Biomaterials Biomaterials and bio-inspired nanomaterials are an obvious area of need for enhanced imaging capabilities. Drying artifacts in conventional EM invariably alter the system, and liquid-based EM lacks contrast and resolution and has enhanced influence of the e- beam due to electrolysis in solutions. Assembly of complex biomimetic materials and the incorporation of functional nanomaterials is a major area of interest for CINT and its users, and improved imaging of these materials and their interfaces is of tremendous benefit.

Soft Materials The organization of soft matter into complex architectures can also be probed, including micelles, liposomes, and polymersomes, as well as microphase separation of polymeric materials. Cryo EM is critical for these materials, and Cryo FIB will allow for a full understanding of the three dimensional arrangement of unperturbed structures.

Nanoparticles and Nanocomposites Observing nanoparticles in vitrified samples allows for direct investigation of nucleation and growth, providing a unique opportunity to probe the very early stages of formation. Self- and directed-assembly (e.g. DNA or polymer directed) of nanoparticle composites in solution can be investigated, as well as the assembly and surface structure of surfactant layers, leading to tremendous gains in knowledge about the behavior of nanoparticles in liquid and solid matrices.

Sensitive Materials Lessening the energy deposited by an electron beam is also critically important to in-situ measurements of electrochemically active and low-Z systems like battery materials. The low voltage microscope and cryogenic analysis both minimize beam damage and will complement our existing in-situ measurement capabilities that involve higher kV and electron doses.

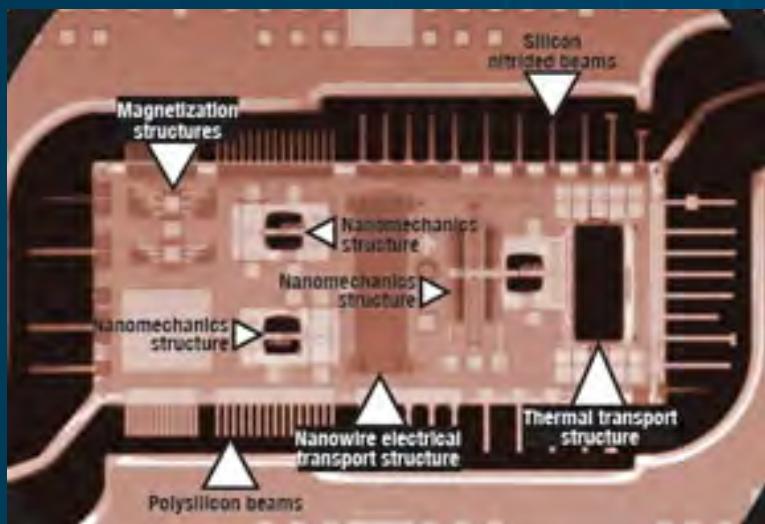
Cost of Cryo Suite: \$2.0M including installation

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Discovery
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Retired Equipment and Areas Deemphasized

Principles:

- 1) Low user interest
- 2) Equipment reached end-of-life
- 3) Limited staffing availability
- 4) Capability becomes main stream and is not a "core capability"



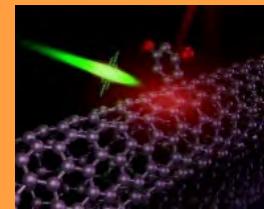
Examples:

- 3 UHV STMs – not productive tools for our user program
Still operate: unique STM capabilities
"Atomic Precision Fabrication – STM".
- One AFM retired – new one installed at Gateway
- Nanomechanics discovery platform not supported anymore. Lack of user requests and new discovery platforms are being developed.
- Old growth furnace salvaged. New 2D materials capability will be built
- Old SEM replaced with new equipment

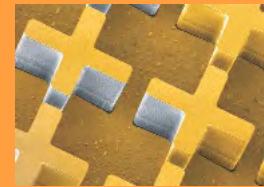
CINT Differentiating Strengths

(1)
(2)
(3)

- Nanomaterials Integration
- Discovery Platforms™: electrochemical platform for TEM, microfluidic for synthesis, NEW: quantum sensed NMR platform to study nuclear spin at the smallest length scales
- Quantum systems:
 - Measuring single spin electron spin resonance and nuclear magnetic resonance quantum dots,
 - Defect centers fabrication, electronic and photonic capabilities for creation of novel qubits
 - Non-adiabatic excited state molecular dynamics codes
- Novel synthetic approaches for heterostructured nanowires, nanoparticles and 2D-materials
- Metamaterials for photonics and optoelectronics
- Ultra-fast and ultra-high resolution spectroscopy of nanomaterial dynamics
- Nanomechanics: understanding of defects/crystal distortions on the mechanical properties
- Hybrid and soft matter and bio-inspired materials
- In-situ microscopies: gaseous and liquid environments, nanomechanics, ion-irradiation (I3SEM, I3TEM)
- Advanced simulation techniques, LAMMPS, and multi-scale theory for interfaces and dynamics, modeling of soft materials

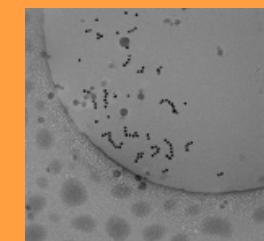
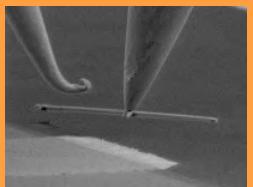


Quantum Systems, III-V Epitaxy & Nanophotonics

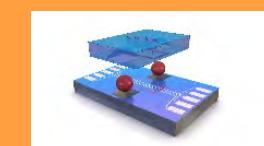


Metamaterials & Ultrafast Spectroscopy

Nano mechanics



Soft Matter & Biomolecular Nanocomposites

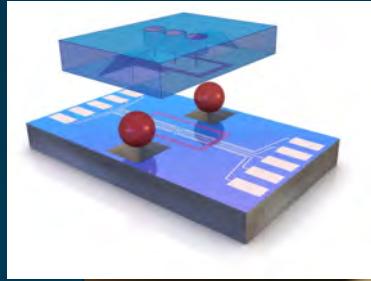


Discovery Platforms

MESA, NHMFL

Ion Beam Labs

Discovery Platforms: microscale modules for the fabrication and study of nanomaterials



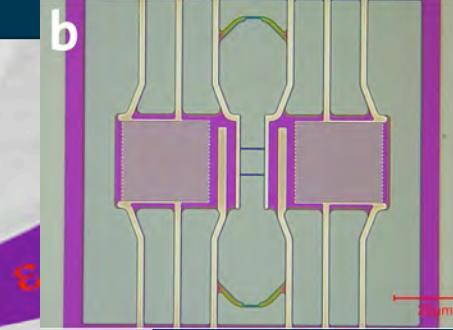
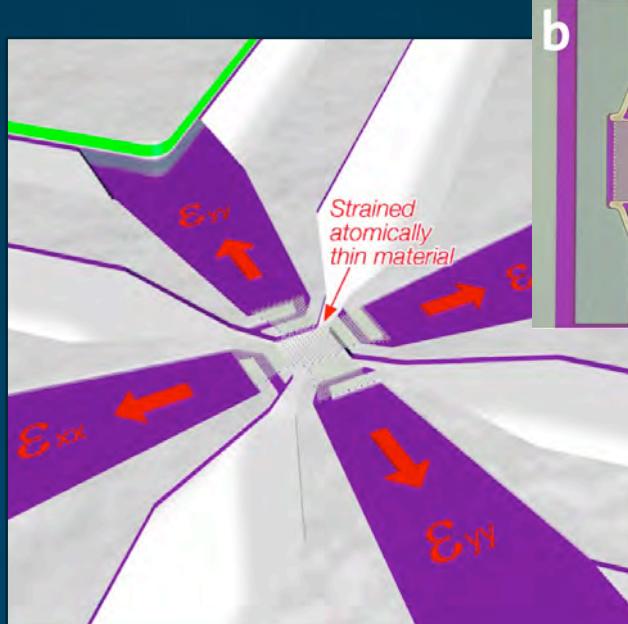
Microfluidics DP

Electrochemical TEM DP

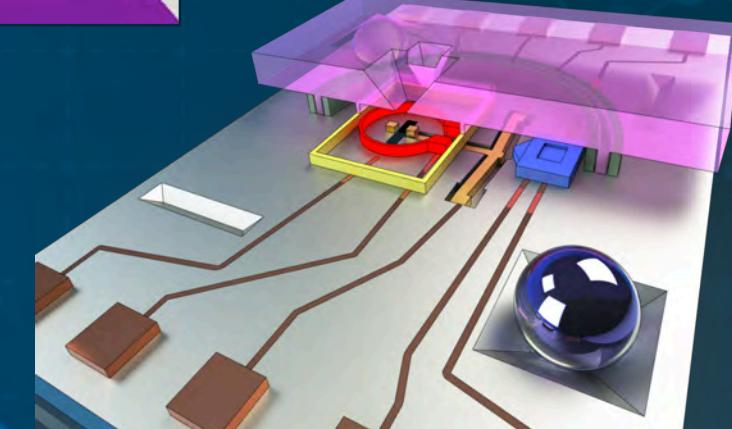
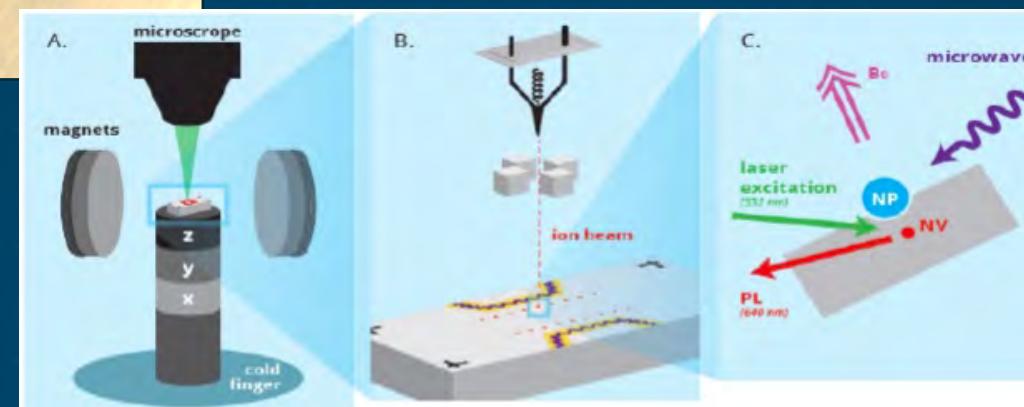
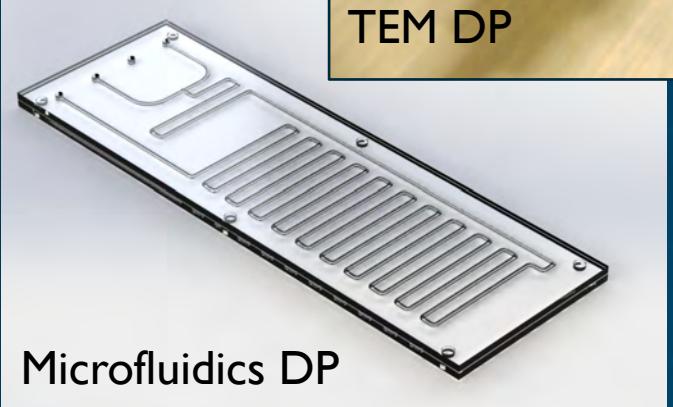
Electrochemical TEM DP



Quantum Sensed NMR DP



Electro-Thermal DP



Mechanical-Environmental-
Thermal MEMS TEM DP

New Staff Hires

Staff



Anastasia Blake



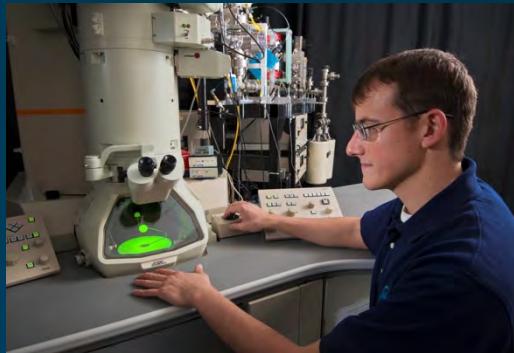
Brad Boyce



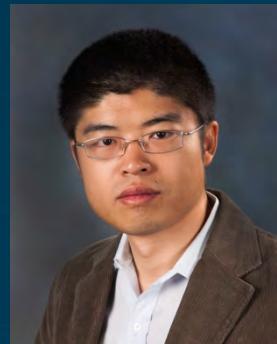
Aiping Chen



Remi Dingreville



Khalid Hattar



Nan Li



Andy Mounce



Michael Pettes



John Watt

Recent Departures:

Nathan Mara (UMN)

Jen Martinez (NAU)

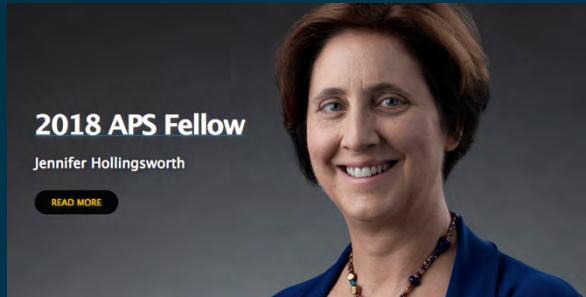
Gabe Montano (NAU)

Wally Paxton (BYU)

We insure staff development especially for early career staff

Staff Recognitions and Awards

Staff



2018 APS Fellow

Jennifer Hollingsworth

[READ MORE](#)

J. Hollingsworth



Jianxin Zhu
Igal Brenner
Jim Werner
Stuart Trugman
Han Htoon
Houtong Chen (OSA)

- 15 elected as society fellows
- 22 society fellowships
- 3 Lab fellows
- Editors on 18 scientific journals
- > 330 invited presentations
- 3 R&D 100 over last 3 years



2018 LANL Fellow

Sergei Tretiak

[READ MORE](#)

S. Tretiak LANL Fellow



S. Doorn LANL Fellow



K. Jungjohann



G. Grest



M. Stevens



I. Brenner



H. Fan



Multifunctional Nanomaterials b
Surfactant-Confined Fabrication

Sandia's 2018
Up & Coming
Innovators.

R&D 100, 2018 for significant
use of LAMMPS code

CINT Users Recognitions and Awards

Users



A. Misra, MRS fellow '16
AAAS fellow '18



Rachel Goldman
UMich Society of Fellows,
Senior Fellow

- National Academy of Inventors
- Royal Academy of Engineering
- FLC award
- 2 DOE Grad Student award
- 2 ThinkSwiss Scholarships
- Distinguished Postdoc awards
- Fellowships, MRS, AAAS



T. Heuser
DOE Graduate Student
Research Award '16



B. Williams
PECASE '16



Q. Jia, National Academy
of Inventors Fellow 2018



J. Driscoll, Royal Academy
of Engineering Fellow 2018



Erika Vreeland, Albuquerque
Business First Women of
Influence

We Support BES Programs Through User Projects



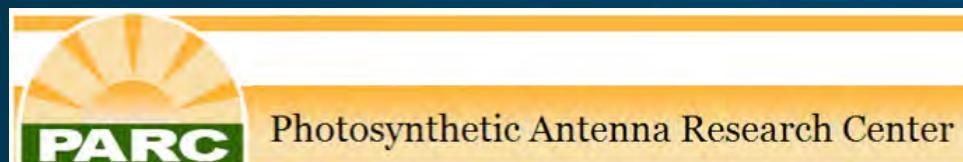
DOE - Hub



CINT supports user from:

DOE-Hubs, EFRCs, BES core programs, EERE, and ARPA-E, early career awardees

EFRCs

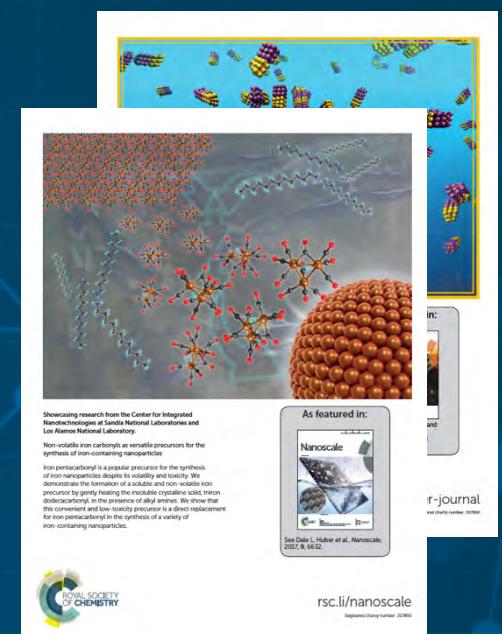
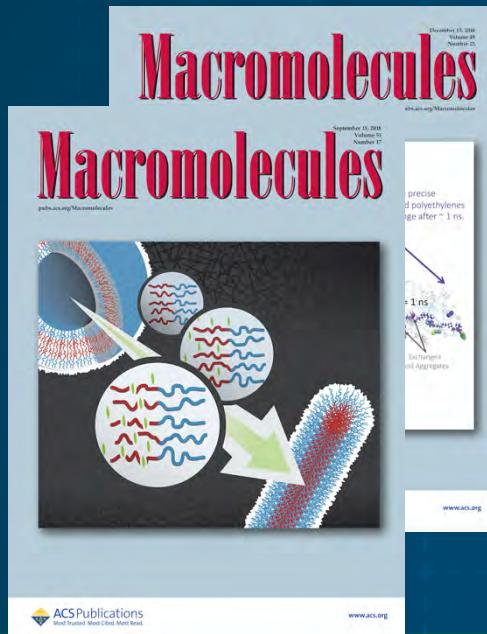
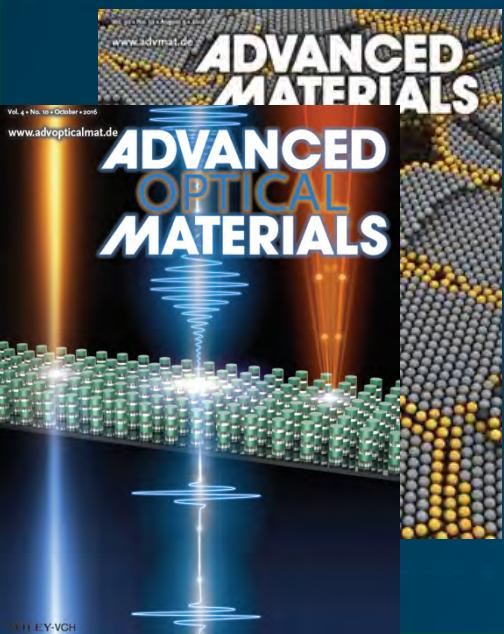
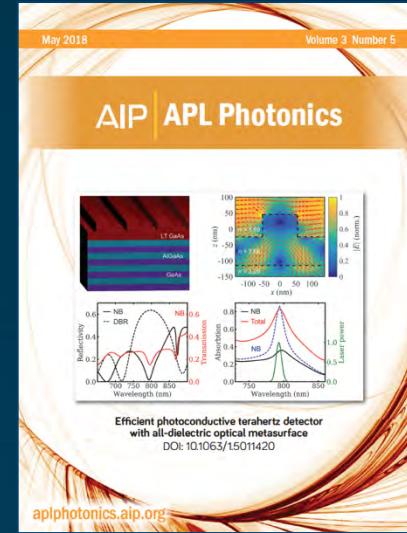
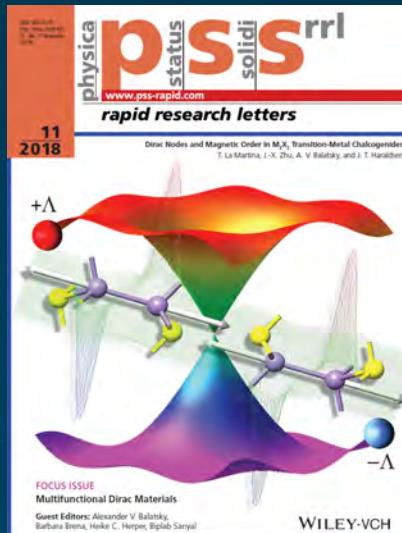
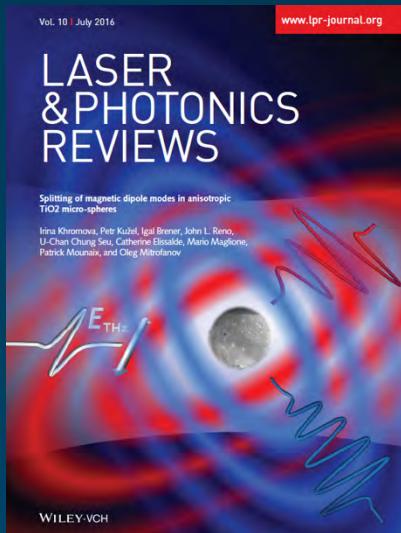
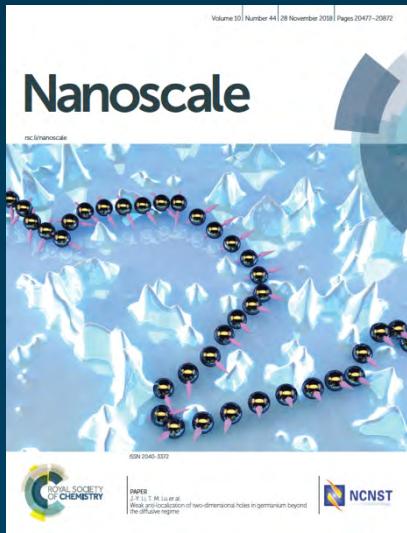
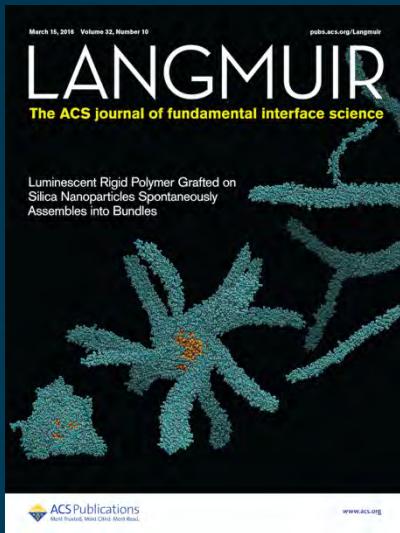
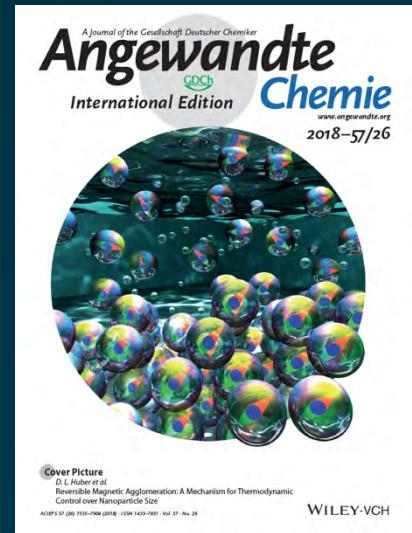


Fundamental Understanding of Transport Under Reactor Extremes



CINT Scientific Leadership

Impact



BES Review Recommendations

Recommendation	Action	Status
(1) Fill co-director vacancy	<ul style="list-style-type: none">Position filled Nov 2016Co-director accepted position as CNMS director Jan 2019New search in progress, targeted completion date July 2019	On-track
(2) Refresh SAC, increase SAC-UEC interactions	<ul style="list-style-type: none">Four new SAC membersNew SAC chairUEC chair ex-officio member of SAC	Done/Continuing
(3) Publication stretch goals	<ul style="list-style-type: none">Expanding staff appointments in strategically identified areas (QIS, cryo-imaging) as well as expanding capabilities (cryoEM suite)Significant increase in publication numbers (19%)	On-track

BES Review Recommendations



Recommendation	Action	Status
(4) Annual recapitalization and carryover investment	<ul style="list-style-type: none">• Recapitalization goal met or exceeded during the current review period• FY19 recapitalization (cryoEM capability) on-track	Done/Continuing
(5) Evaluate safety program	<ul style="list-style-type: none">• ES&H professionals hired at Core• Peer visits and internal audits across both facilities	Done/Continuing
(6) Increase geographical diversity of users and industrial user base	<ul style="list-style-type: none">• New Communications and Outreach Manager• Targeted outreach at top-publishing materials science departments• Increased industrial representation on SAC, UEC and PRC	On-track
(7) Integrate theory across facilities and user base	<ul style="list-style-type: none">• Restructured scientific thrusts to better integrate theory	Done/Continuing

Key Message

- 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





BIG SCIENCE AT THE NANOSCALE

CINT is a user facility providing cutting-edge nanoscience and nanotechnology capabilities to the research community.

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