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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

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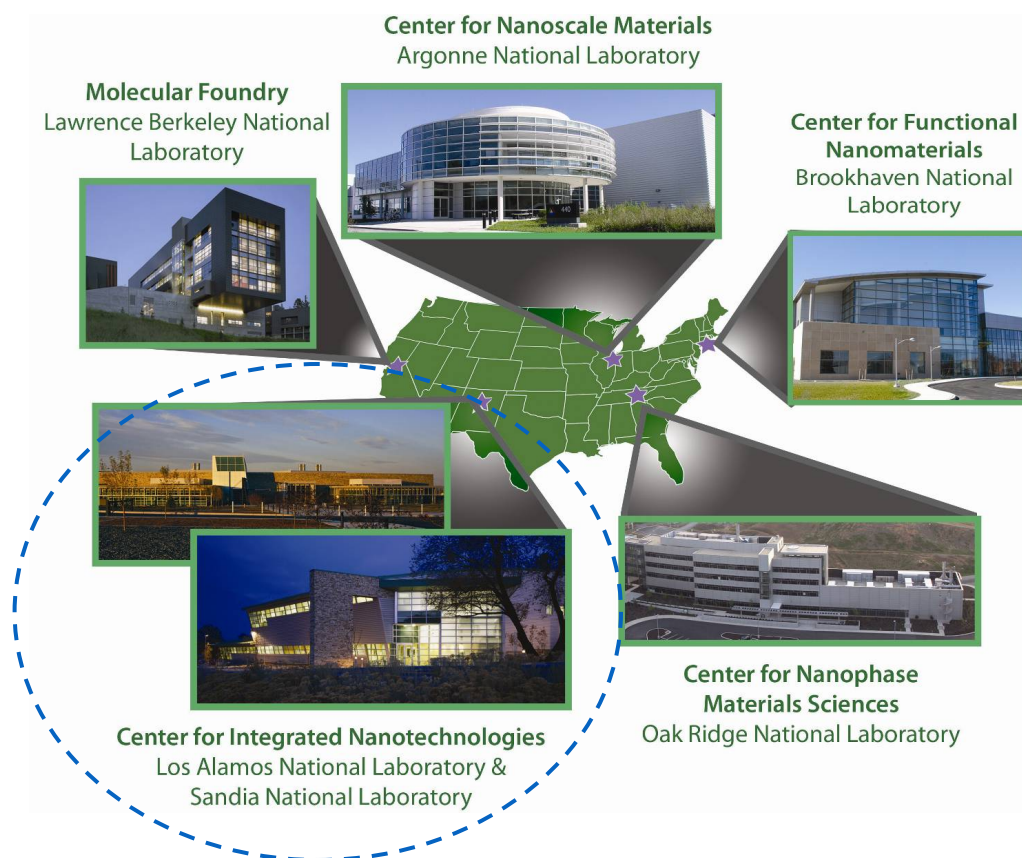


- CINT's vision, mission, and structure
- Host labs capabilities and connections
- Environment, Safety and Health
- Differentiating capabilities in nanoscience
- Growth in user community, productivity, and scientific impact
- Brief future opportunities and outlook
- Response to BES recommendations of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

# CINT is a DOE Office of Science National User Facility



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



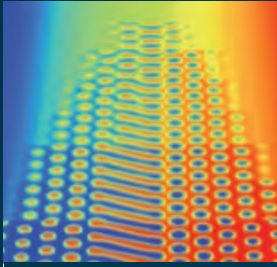
The DOE/SC nanoscience centers are different from traditional user facilities

- 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





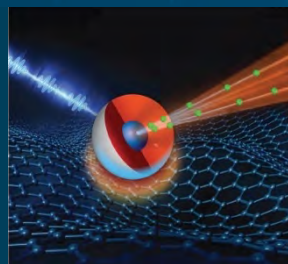
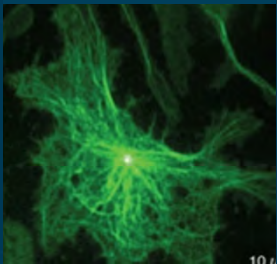
## User Mission

*Provide users with world-leading scientific expertise and capabilities*



## Scientific Mission

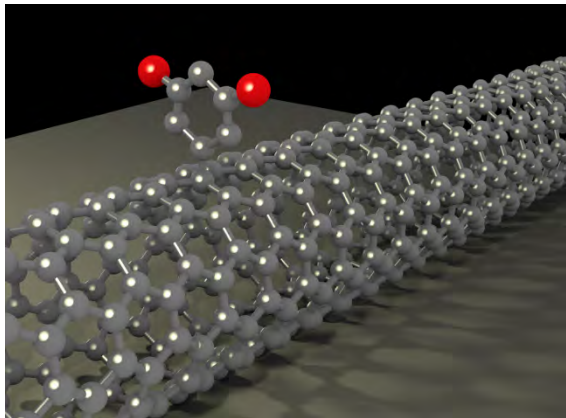
*Provide scientific understanding underlying nanoscale integration through the assembly of diverse materials across multiple length scales, with the ultimate goal to design and control new material properties and functionality*



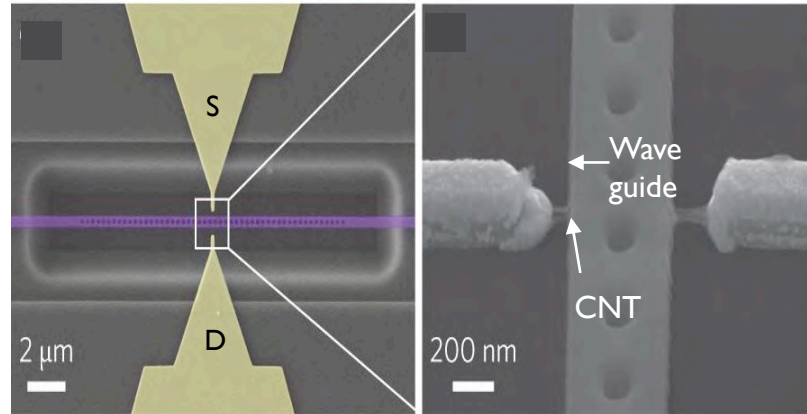
## Scientific Thrusts

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

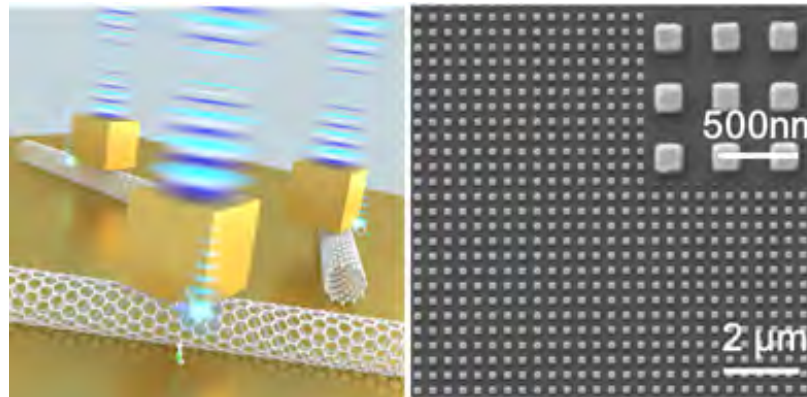
# Concept of Integrated Nanotechnologies



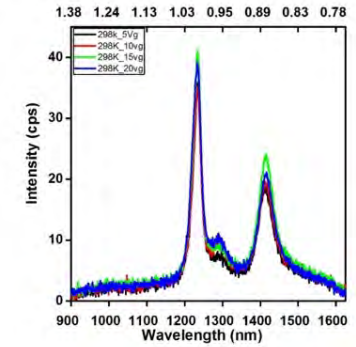
Functionalized Nanotube



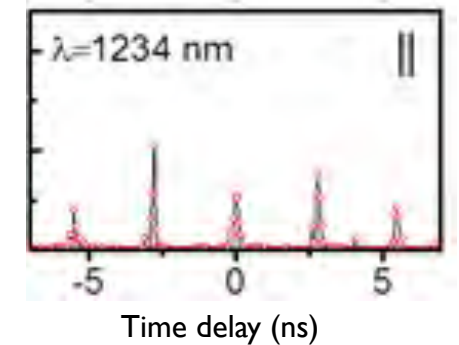
Nanotube Field Effect Transistors



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



# CINT Provides User Access to Significant Capabilities at both Host Institutions



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

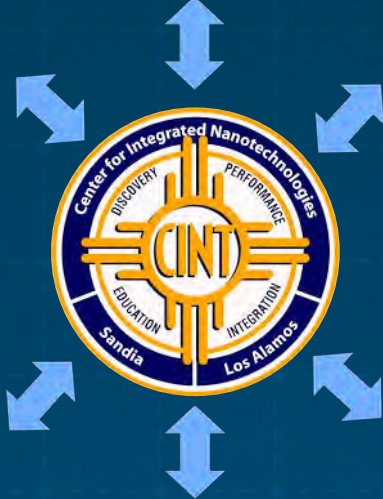


Ion Beam Labs (SNL and LANL)

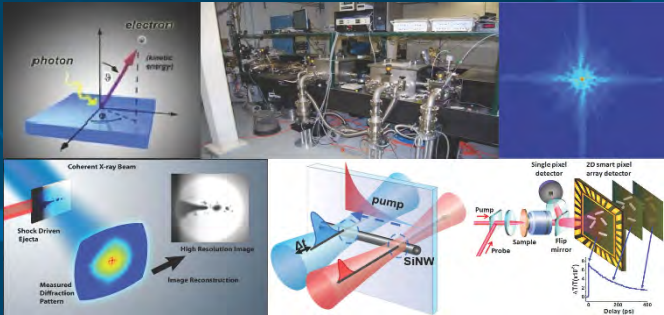
National High Magnetic Field Laboratory (LANL)



Los Alamos Neutron Science Center (LANSCE) (LANL)



High Performance Computing (SNL and LANL)



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



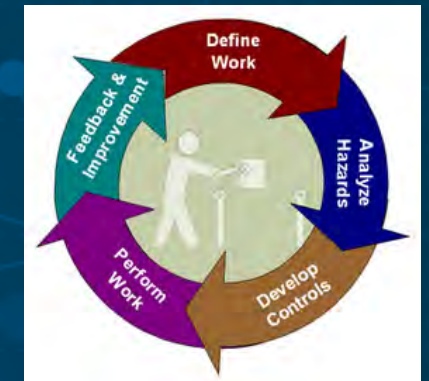


## Integrated Safety Management (ISM)

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

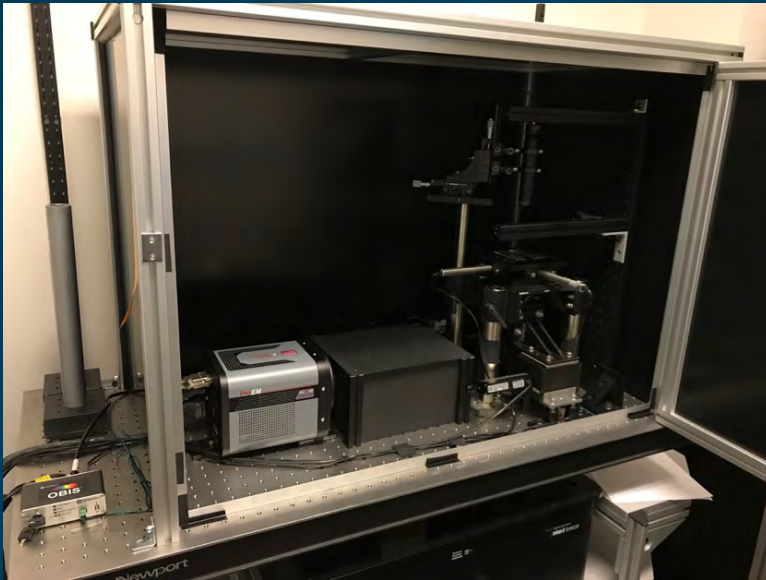
- Exposure Assessments
- Medical Surveillance Programs
- Safety Training
- Waste Management  
includes pollution prevention, waste minimization



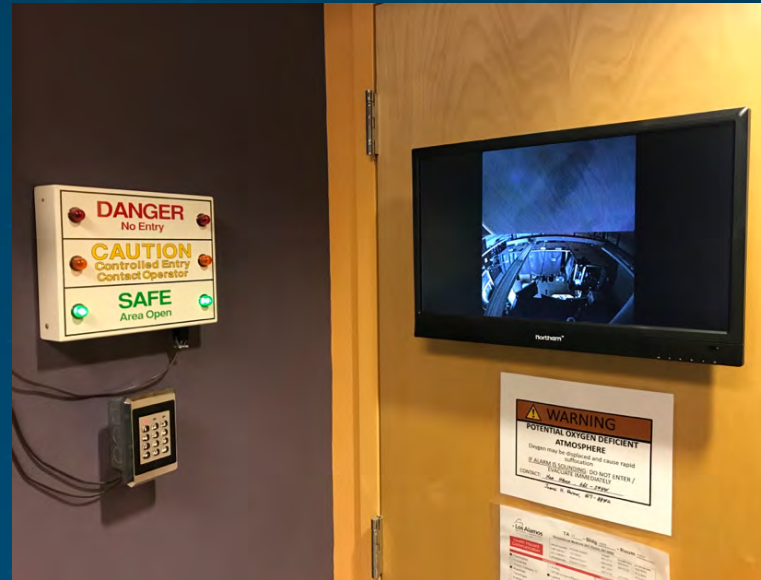


## CINT is committed to safety and security

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

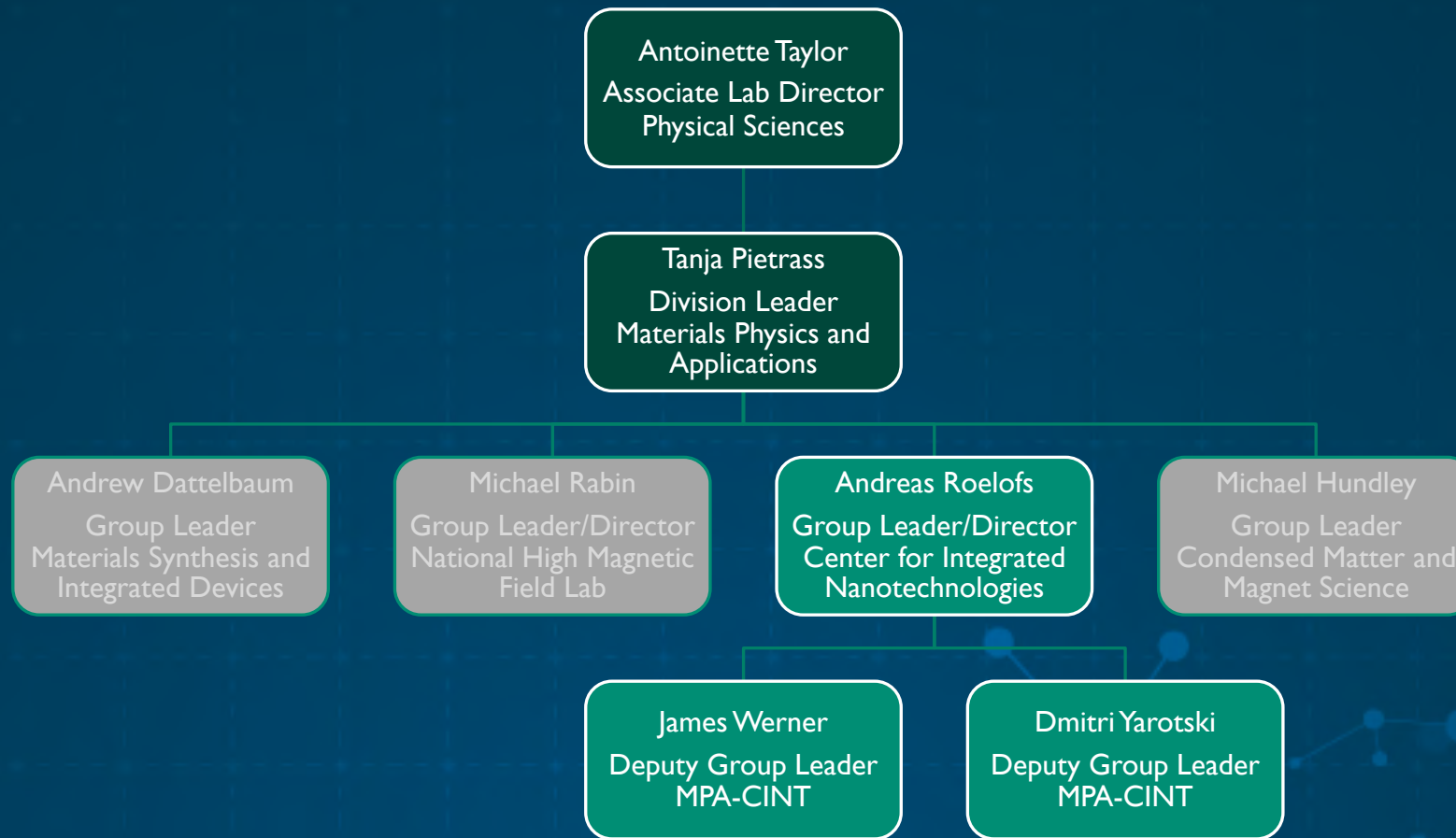


Engineering control

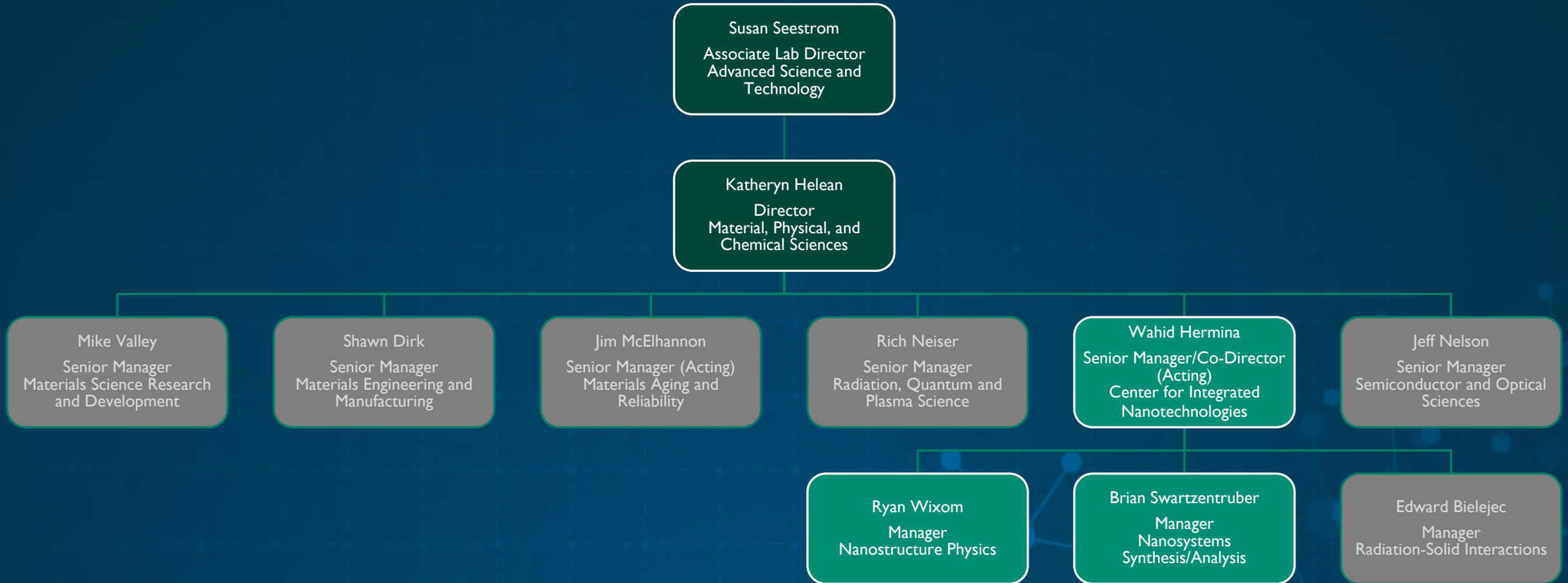


Best practice: virtual windows

# LANL Organizational Chart

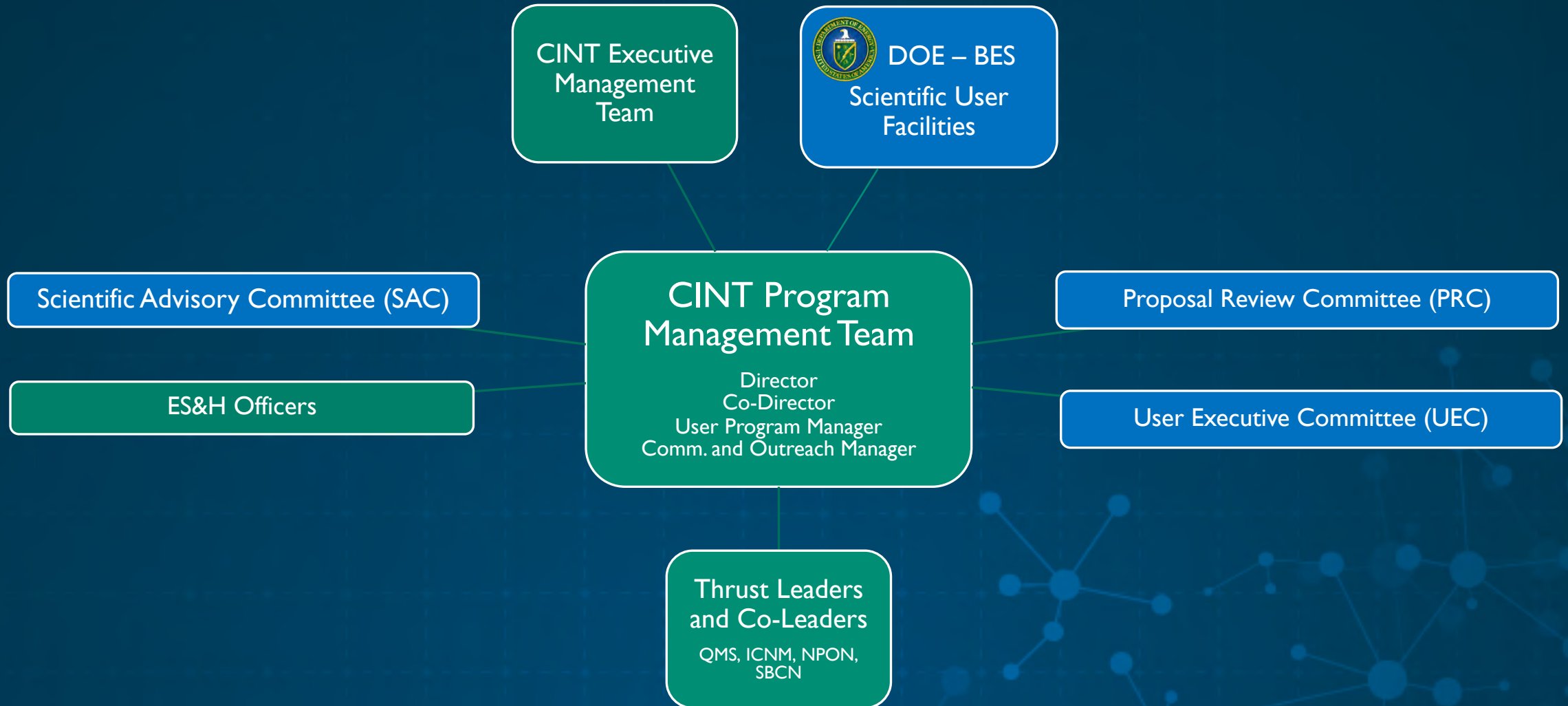


# Sandia Organizational Chart

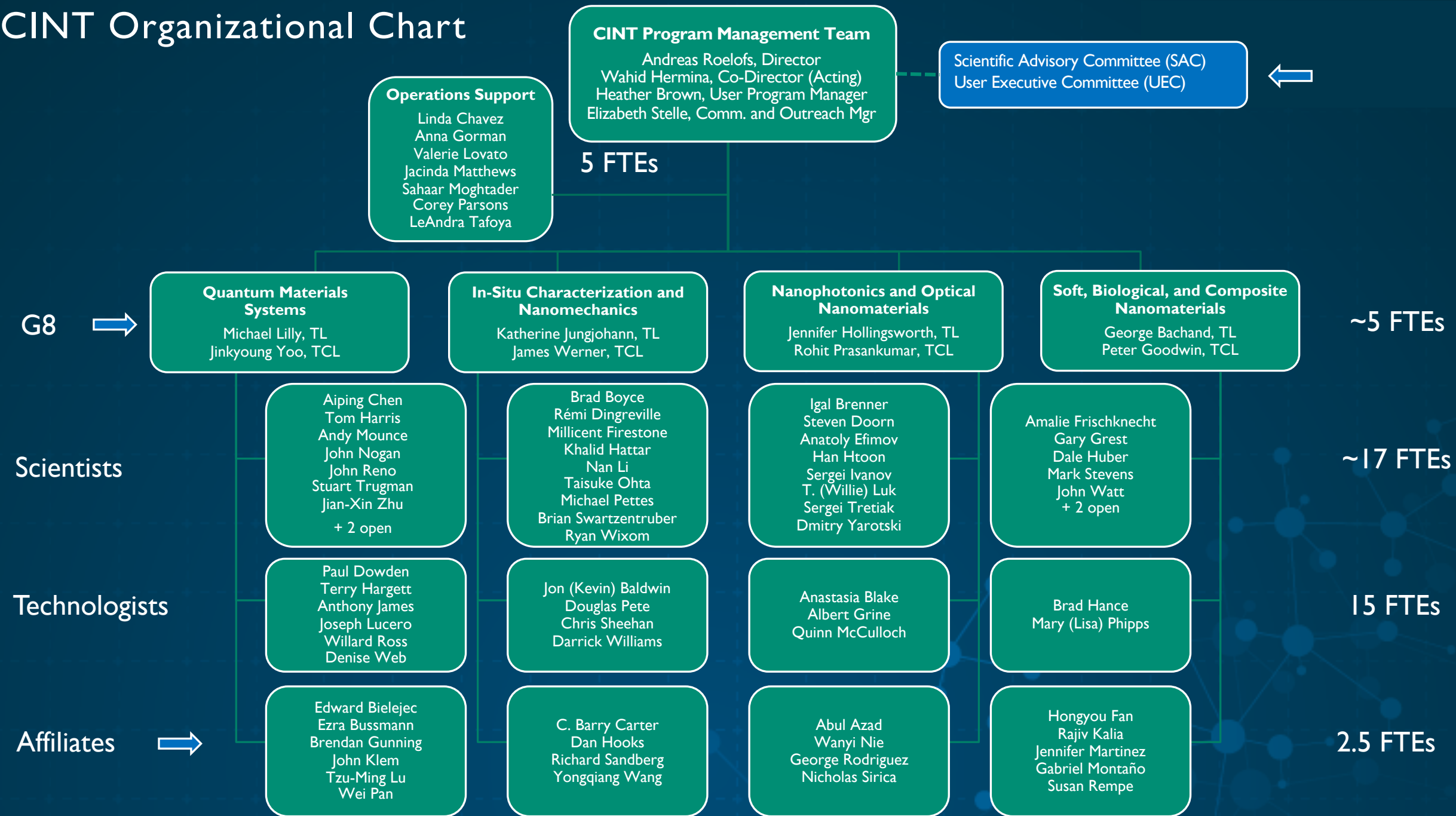




# CINT High-level Organizational Chart



# 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

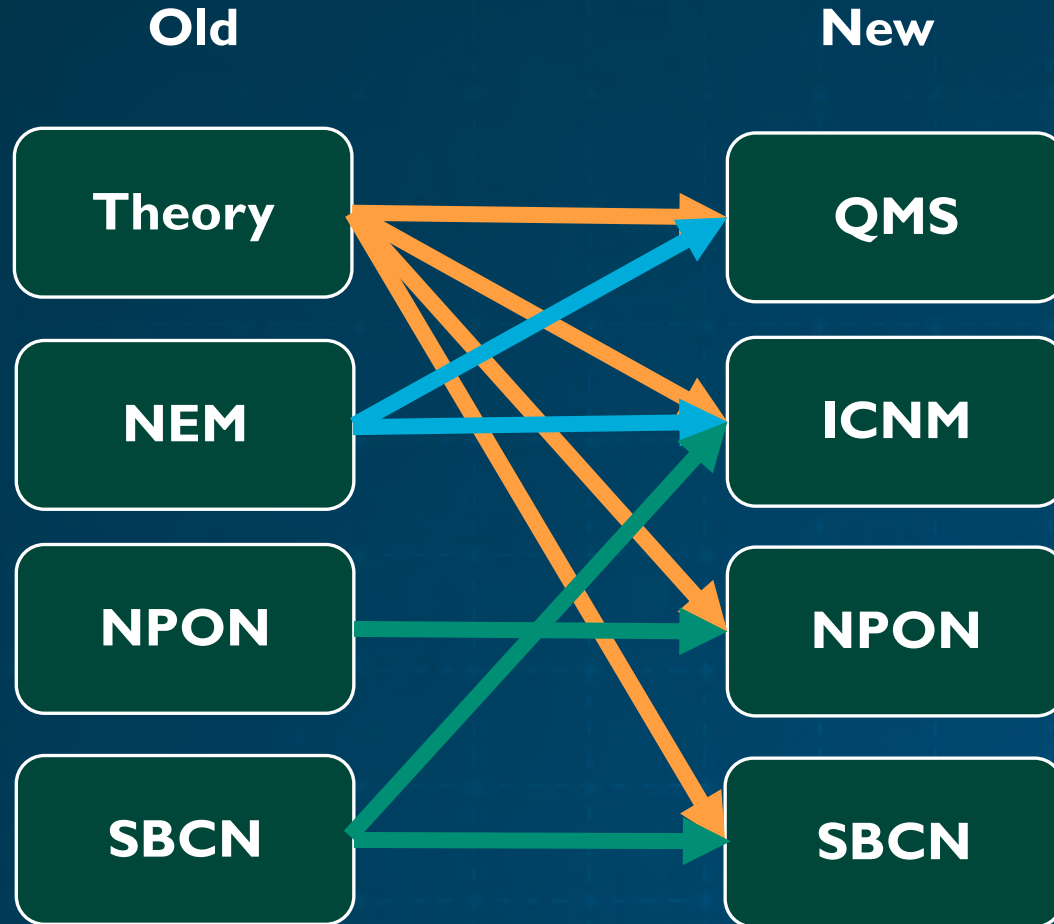
- New Chair: Rachel Goldman
- 4 new members
  - Shef Baker, Cornell University
  - Judith Driscoll, University of Cambridge
  - Rachel Goldman
  - Jim Hannon, IBM
- Julia Fulghum, former Chair, rotated off after serving for 5 years.
- UEC Chair joined SAC

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

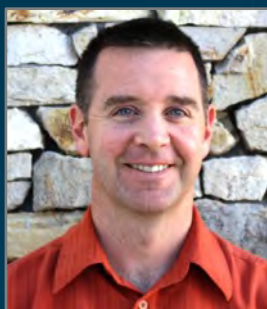
NPON: Nanophotonics and Optical Nanomaterials  
SBCN: Soft, Bio and Composite Nanomaterials  
ICNM: In situ Characterization and Nanomechanics  
QMS: Quantum Materials Systems

# CINT Science Leadership Team (“G8”)



## Quantum Materials Systems

### Thrust Leaders



Mike Lilly

## Nanophotonics and Optical Nanomaterials



Jen Hollingsworth

## Soft, Biological, and Composite Nanomaterials



George Bachand

## In-situ Characterization and Nanomechanics



Katie Jungjohann

### Thrust Co-Leaders



Jinkyong Yoo



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

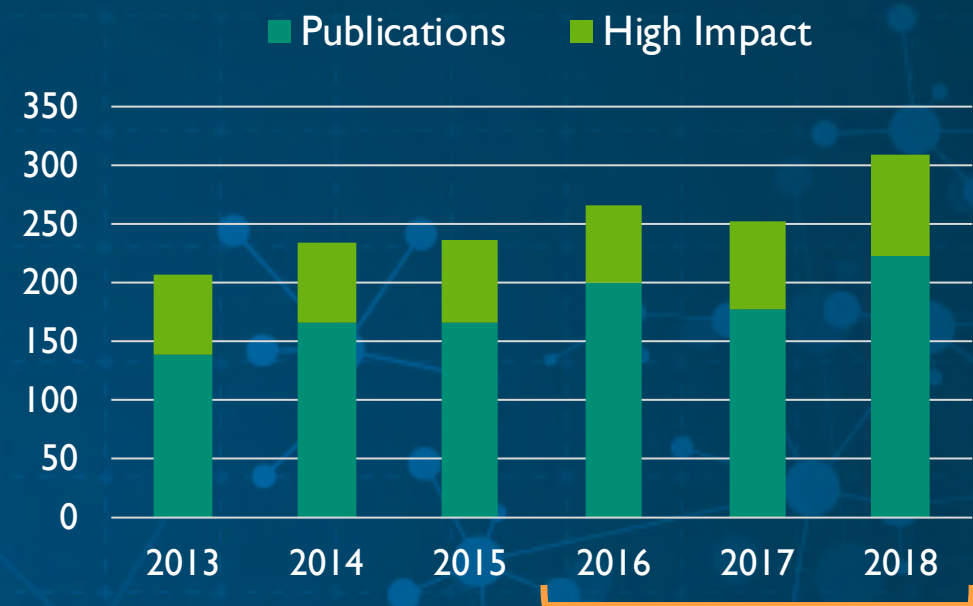
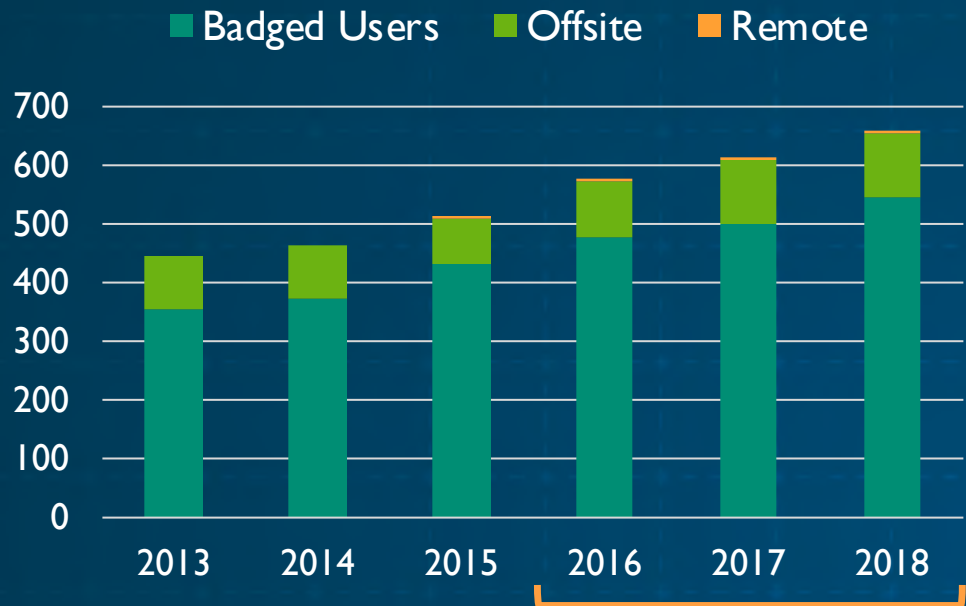
Rec #3 publication goal

**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

## Capabilities



## Rec #4 10% Recapitalization

2016

- 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

2017

- 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

2018

- 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

2019

- 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



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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      Aquilos 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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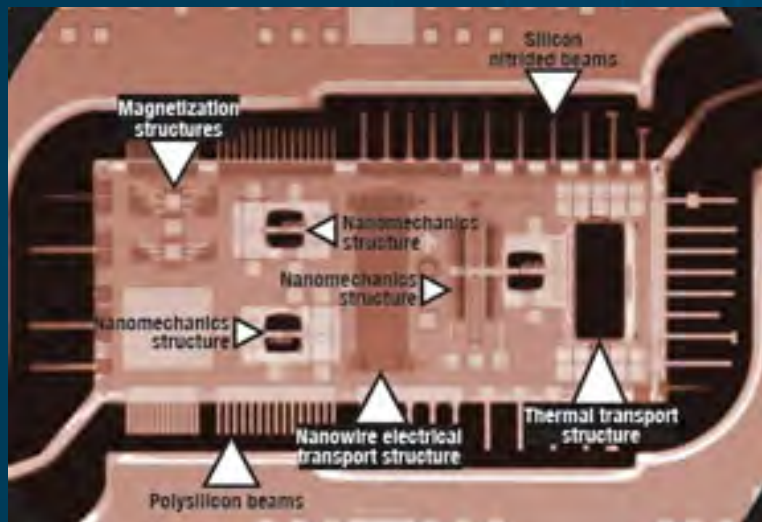
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# Retired Equipment and Areas Deemphasized

## 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"



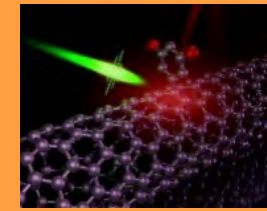
## Examples:

- 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

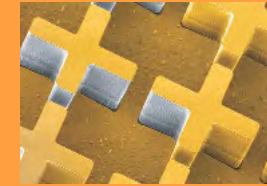
- Nanomaterials Integration
- Discovery Platforms™: electrochemical platform for TEM, microfluidic for synthesis, NEW: quantum sensed NMR platform to study nuclear spin at the smallest length scales
- Quantum systems:
  - Measuring single spin electron spin resonance and nuclear magnetic resonance quantum 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



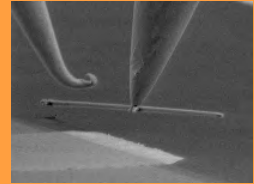
**Quantum Systems, III-V  
Epitaxy & Nanophotonics**



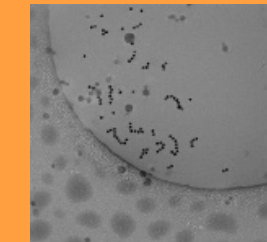
**Metamaterials  
& Ultrafast  
Spectroscopy**



**Nano  
mechanics**



**Soft Matter & Biomolecular  
Nanocomposites**



**Discovery  
Platforms**

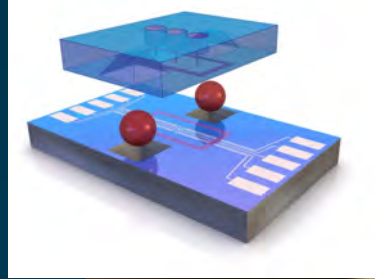


**MESA, NHMFL**

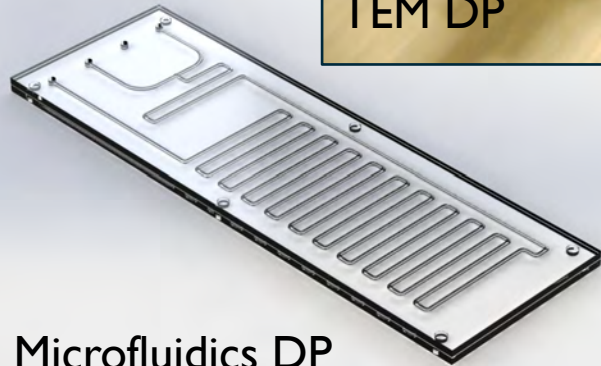
**Ion Beam Labs**



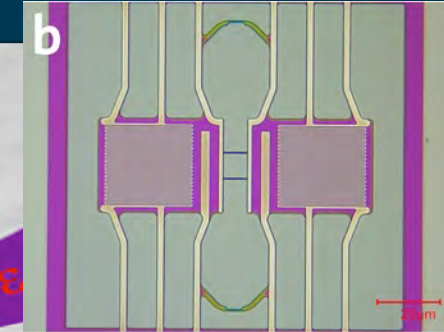
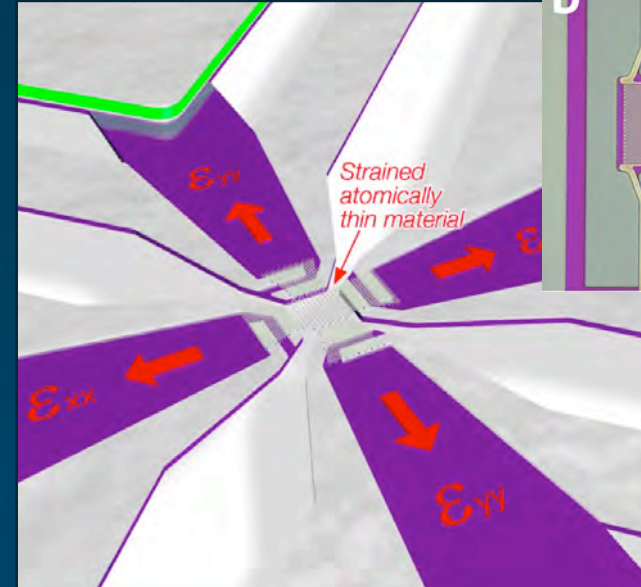
# Discovery Platforms: microscale modules for the fabrication and study of nanomaterials



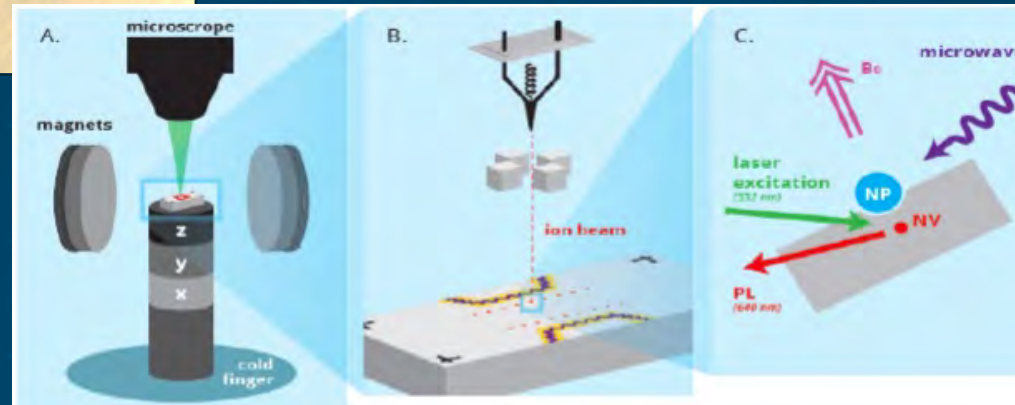
Electrochemical  
TEM DP



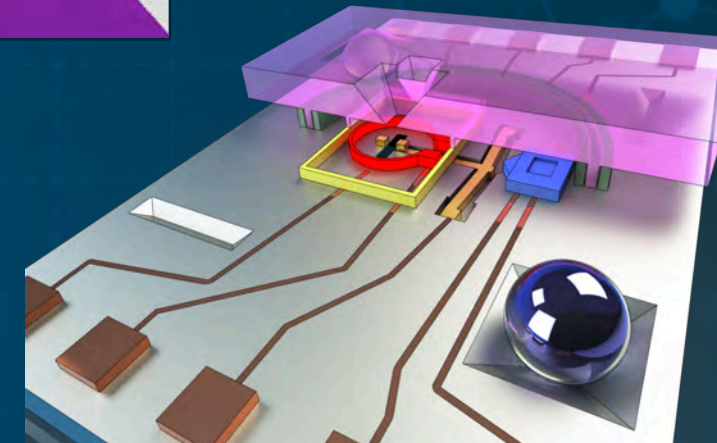
Microfluidics DP



Electro-Thermal DP



Quantum Sensed NMR DP



Mechanical-Environmental-  
Thermal MEMS TEM DP

# New Staff Hires

Staff



Anastasia Blake



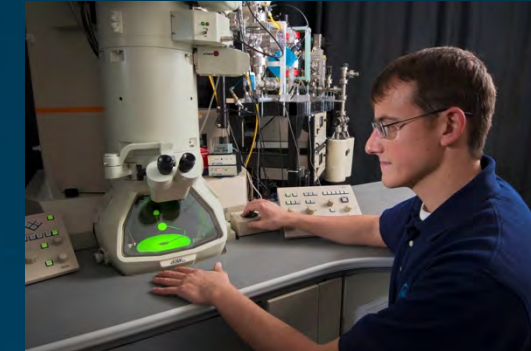
Brad Boyce



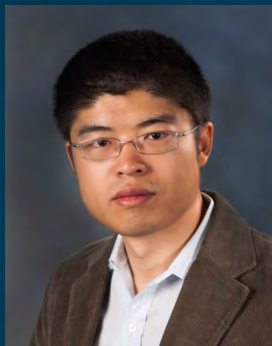
Aiping Chen



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

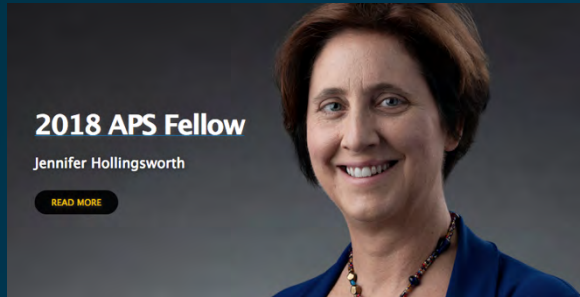


# Staff Recognitions and Awards

Staff



Los Alamos  
NATIONAL LABORATORY  
EST. 1943



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

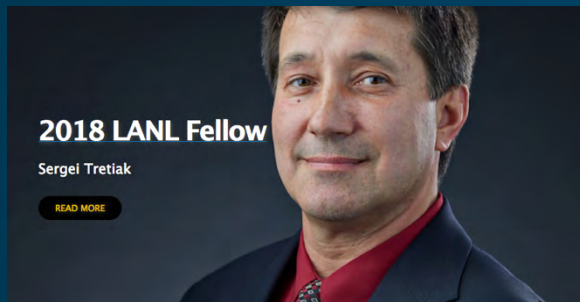


I. Brenner

Sandia's 2018  
Up & Coming  
Innovators.

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

Multifunctional Nanomaterials b  
Surfactant-Confined Fabrication



S. Tretiak LANL Fellow



S. Doorn LANL Fellow



K. Jungjohann



G. Grest



M. Stevens



H. Fan



# CINT Users Recognitions and Awards

Users

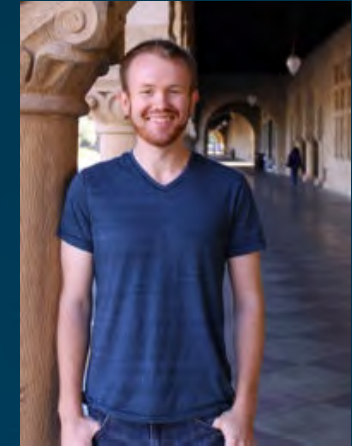


A. Misra, MRS fellow '16  
AAAS fellow '18



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

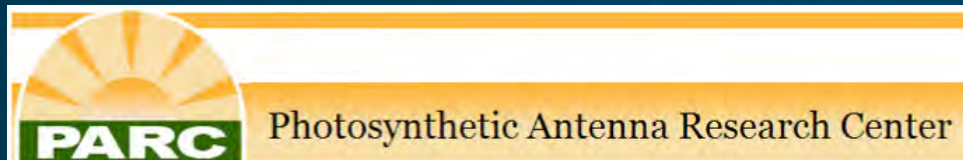
## DOE - Hub



### CINT supports user from:

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

## EFRCs



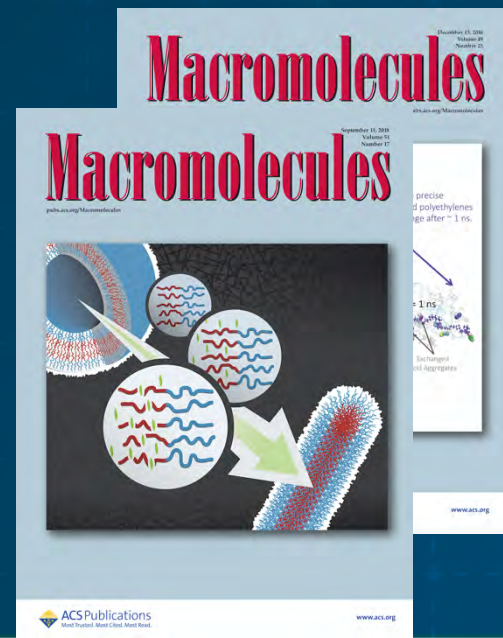
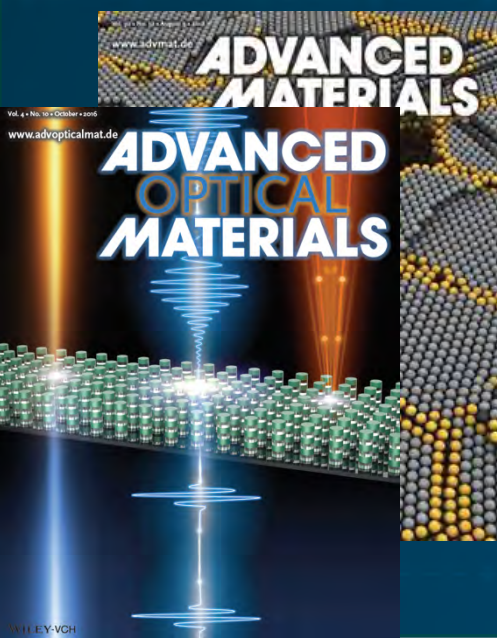
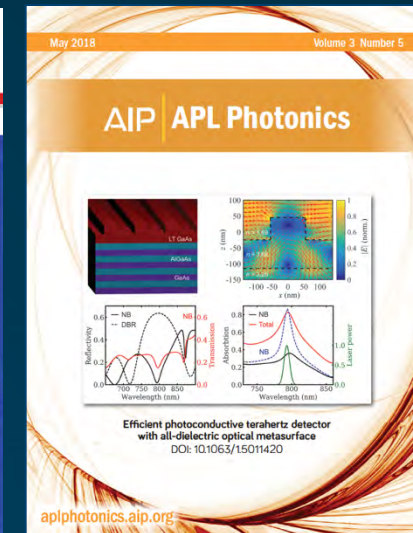
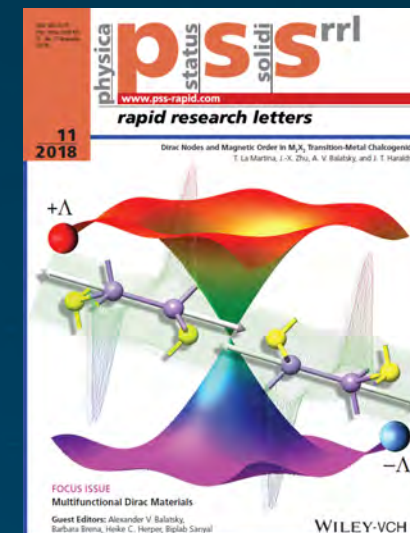
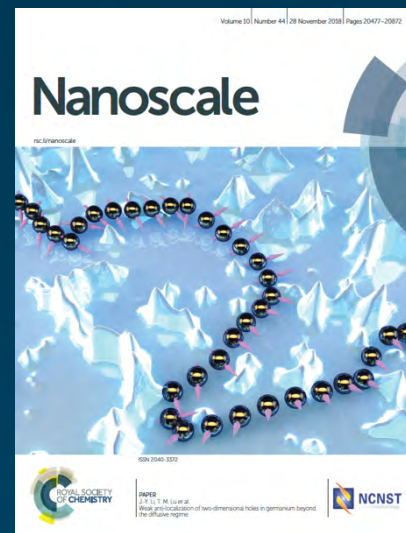
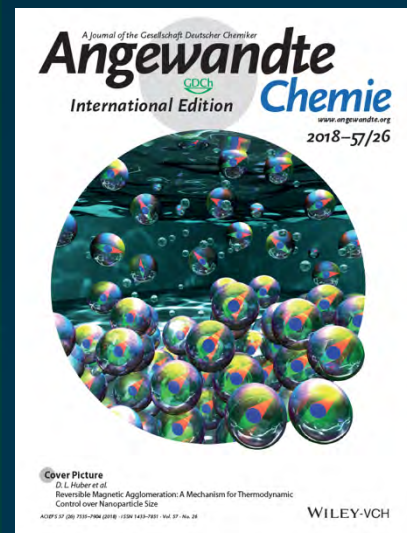
Fundamental Understanding of  
Transport Under Reactor Extremes





# CINT Scientific Leadership

Impact





# BES Review Recommendations

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

# BES Review Recommendations

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

Center for Integrated Nanotechnologies  
– an Office of Science national user facility –

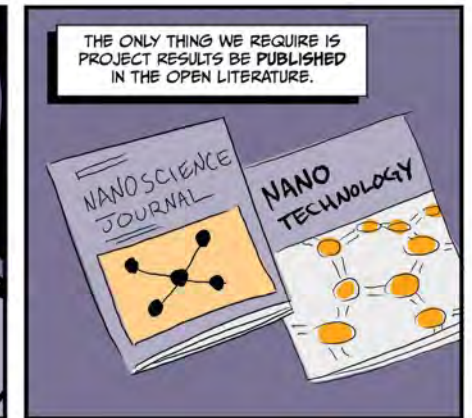
**CINT** is a user facility providing cutting-edge nanoscience and nanotechnology capabilities to the research community.

Access to our facilities and scientific expertise is **FREE** for non-proprietary research.

## Research areas:

- Quantum Materials Systems
- Nanophotonics and Optical Nanomaterials
- In-Situ Characterization and Nanomechanics
- Soft, Biological, and Composite Nanomaterials

To learn more and  
apply to use the facilities, visit:  
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