



SAND2016-4188PE

CINT the Next Decade

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(acting) CINT Co-Director
May 10-12, 2016



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.



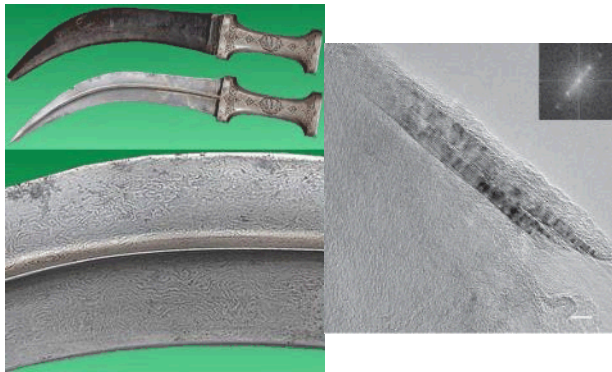


Overview

- **Integrations role in nanotechnology**
- **Forefronts of nanotechnology**
- **CINTs Strategic plan**
 - **Three focus areas**
 - **Current and future capabilities**



Nanotechnology Throughout History

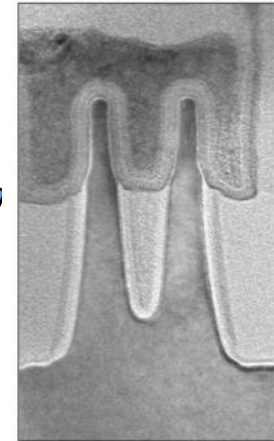


Carbon nanotubes in 17th Century
Damascus steel

Reibold, et. al, Nature 444, 286 (2006)



Motorola i870 (2005)
- Ag nanoparticle
antimicrobial coating



Intel 14nm
Broadwell CPU
(2015) ~26 Atoms

It is the integration of nanostructures that made these impactful



CINT's Vision

CINT (2004)



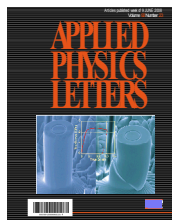
CINT's Core and Gateway (today)



“To be the **national resource** for research expertise and advanced capabilities to synthesize, fabricate, characterize and understand the **integration of nanostructured materials.**”



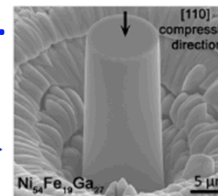
Leveraging Host Institutions' Capabilities Important for User Community and BES Programs



Appl. Phys. Lett. 92, 231901 (2008).

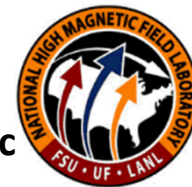
Nanomechanics facility established at CINT

Acta Mater. 60, 5670 (2013).



Magnetic shape memory alloys

Leveraging High Magnetic Field Laboratory at LANL

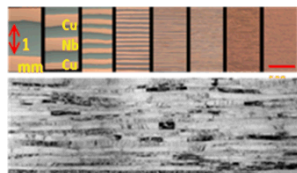


2006

BES Programs leveraged Nanomechanics at CINT:

- CMIME EFRC
- Core Programs

Bulk Nanocomposites



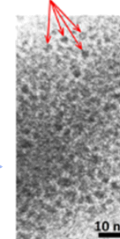
Nat. Comm. 4, 1696 (2013).

Leveraging Ion Beam Materials Lab at LANL



2015

Helium bubbles

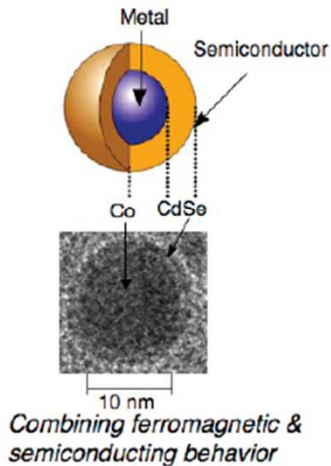


Nano Lett. 14, 5176 (2014).

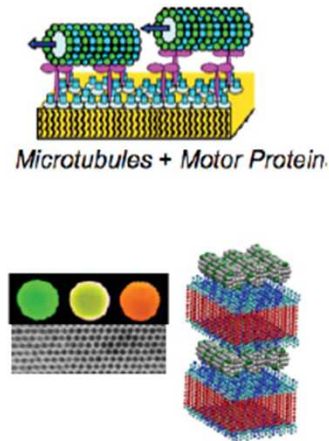


Integration Across Length Scales

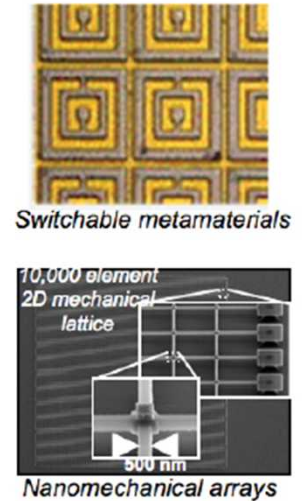
Nano materials



Nano assembly



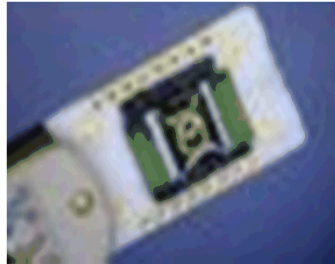
Larger nanosystems



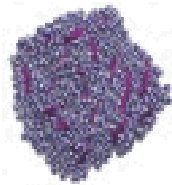


CINT's World-leading Capabilities

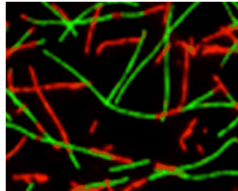
**Discovery
Platforms**



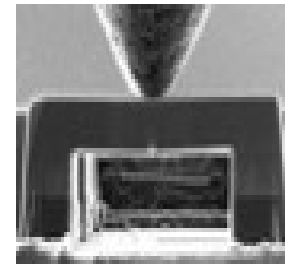
**Metamaterials
& Ultrafast
Spectroscopy**



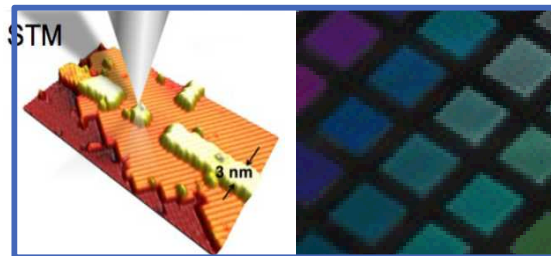
**Soft Matter & Biomolecular
Nanocomposites**



**Five World-
leading
Capabilities**



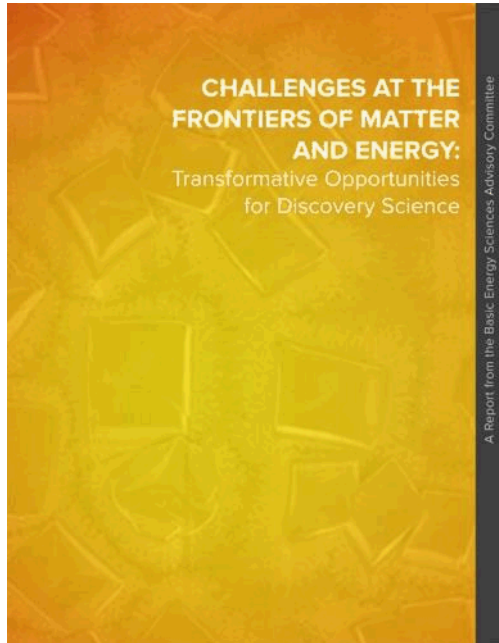
**Nano
mechanics**



**Quantum Systems &
III-V Epitaxy**



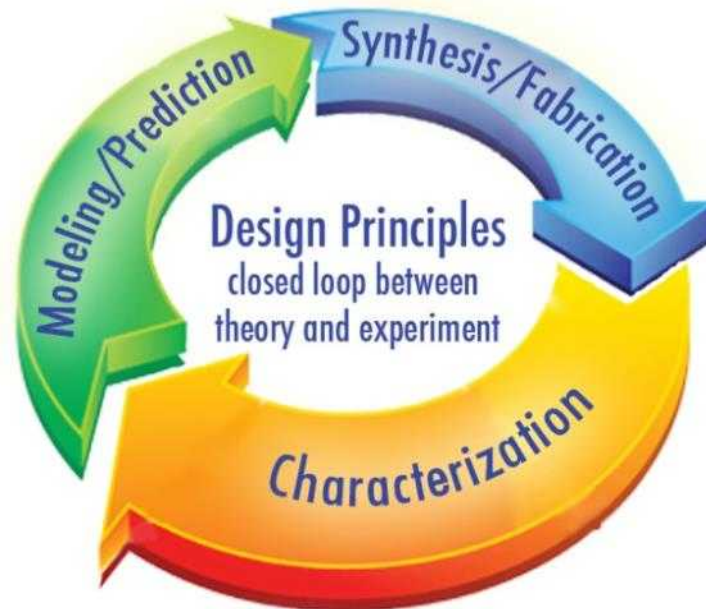
The Challenges to Nanotechnology



2015 BESAC report

The Frontiers:

1. **Predictive models**, including the incorporation of metastability, to guide the creation of beyond-equilibrium matter;
2. Mastering **synthesis and assembly of hierarchical structures** for multidimensional hybrid matter; and
3. **In situ Characterization** of spatial and temporal evolution during synthesis and assembly.





Our Strategic Planning Process

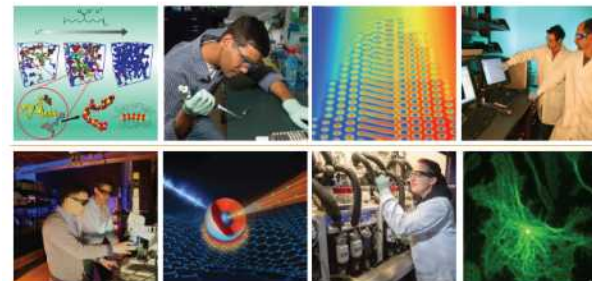
CINT Thrust Leaders, Partner Science Leaders, and Management conduct strategic planning via regular meetings and special dedicated off-site events.

Input from:

- CINT Scientists & users
- Annual CINT User Conference
- Joint NSRC technical workshops
- LANL & SNL institutional plans
- DOE/SC/BES strategic directions
- Science Advisory Council
- User Executive Committee



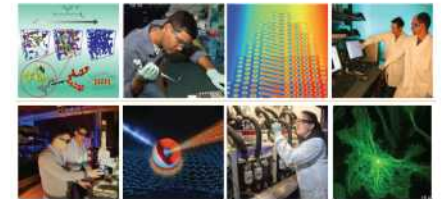
The Center for Integrated Nanotechnologies
Strategic Plan





CINT's Strategic Objectives

1. National leader in nanomaterials integration.
2. Develop unique experimental and theoretical capabilities to synthesize, fabricate, characterize, and understand nanoscale materials.
3. Develop next generation Discovery Platforms.
4. Provide foundational capabilities and commercial instrumentation necessary for internationally competitive nanoscience research.
5. Operate safely and effectively.
6. Increase the diversity and breadth of our national user community, foster high-impact science, and encourage intellectual risk in basic and use-inspired research.



2010-2015

2016-2020

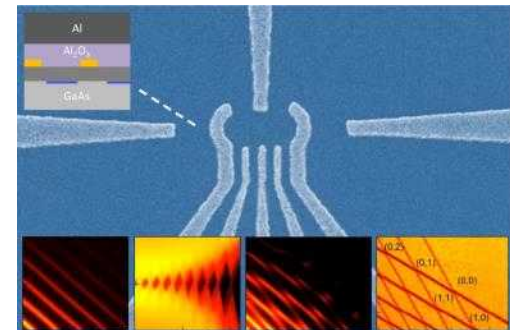




Nanomaterials Integration Challenges

Key challenges to predictable design of hierarchical nano-enabled materials:

1. Understanding and engineering nanoscale electrical and mechanical **nano-scale interfaces**.
2. Hybrid materials interactions for generation and **manipulation of light**.
3. Building **hierarchical** structures & dynamics in **soft matter**.





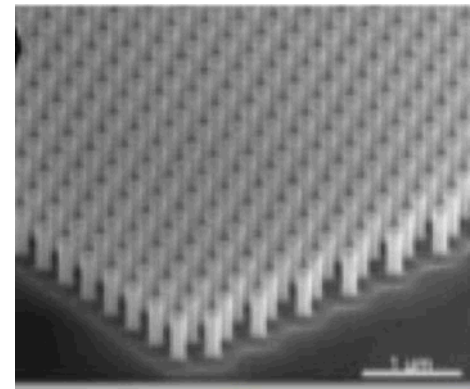
Electrical and Mechanical Integration - Challenge

Scientific opportunity: Scaling-up from isolated nanocomponents to integrate systems still represents a significant challenge.

Issues of Integration

- **Engineering the interface effects between individual nanostructures** in interconnected networks and composite mesoscale structures;
- **Bridging** between emergent **nanoscale functionality to macroscale** performance;
- **Develop geometries** that harness the exceptional axial diffusion behaviors of 1D systems;
- **Determining the ion and electron transport** behaviors at the junctions of nanostructures.

All of these challenges are based on interactions at interfaces.



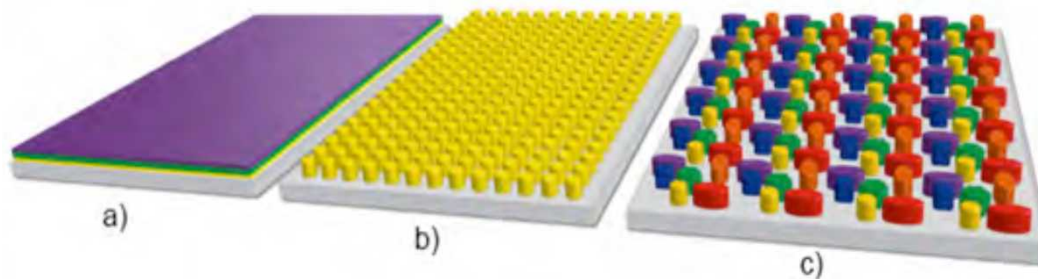


Nanoscale Interfaces – CINT’s Directions

Toward the future: CINT’s ultimate goal is to develop a fundamental predictive understanding of the interfacial interactions between nanoscale components with 0D - 3D confinement.

Challenges

1. Integration and “up-scaling” methodologies for **transforming 1D nanowires and nanotubes into 2D and 3D architectures** and ensemble systems designed for advanced functionality.
2. **Innovation in nanofabrication and integration of the growth of arbitrary, 3D, multifunctional, quantum-size structures.**



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



Nanoscale Interfaces - Capabilities

Current world-leading capabilities:

- MBE growth of high-mobility III-V planar heterostructures;
- Atomic Precision Fabrication;
- Discovery Platform for in-situ TEM measurements.

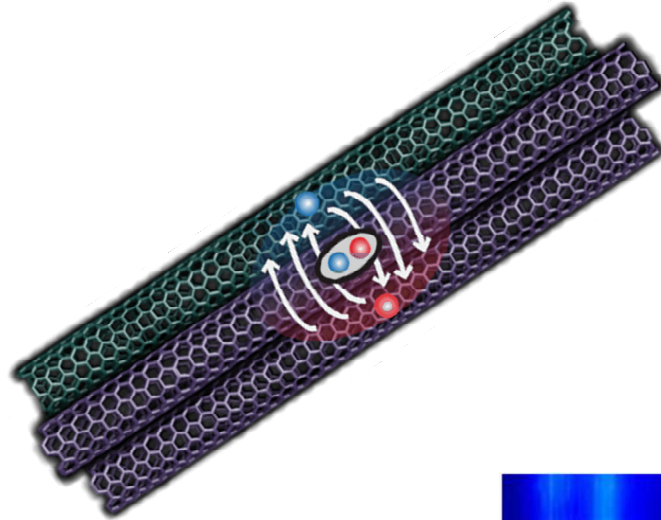


Future Capabilities:

- Expand high-quality growth in Group IV, III-Nitrides, and low-band-gap materials (e.g, InGaAs/InP, antimonides);
- Integrate growth of 0D, 1D, and 2D systems (e.g., quantum dots, nanowires, and thin-films);
- Expand in-situ TEM capabilities in single-interface transport;
- **Develop predictive capability: link between interfacial structure and transport across interfaces;**
- **Develop theory of transport across entire hybrid structures at ensemble scale.**



Hybrid Materials Interactions for Generation and Manipulation of Light



Goal: Engineer and understand new excitations, states, and interactions in composite nanomaterials.

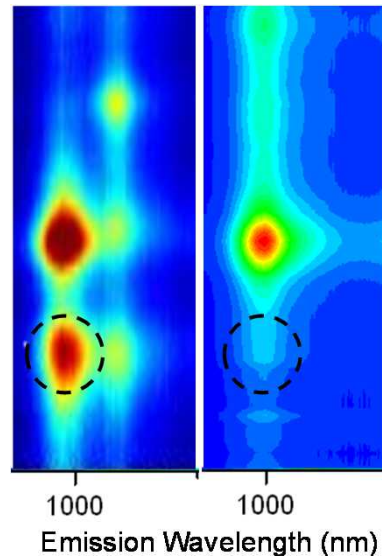
3 Focal Areas:

On demand single photo sources – how to deterministically stimulate single photo emission.

Efficient manipulation of light using nanostructured materials.

Studying new regimes of light mater interactions – combining novel emitters and structures.

- Defining interactions.
- New states and coupling behavior.
- Emergent optical response.





Hybrid Materials Interactions for Generation and Manipulation of Light

Current Capabilities

Characterization:

- Ultra-fast spectroscopy
- Single photo, low temperature, time resolved spectroscopy
- UV to THz spectroscopy
- Low temperature, time resolved Raman

Synthesis:

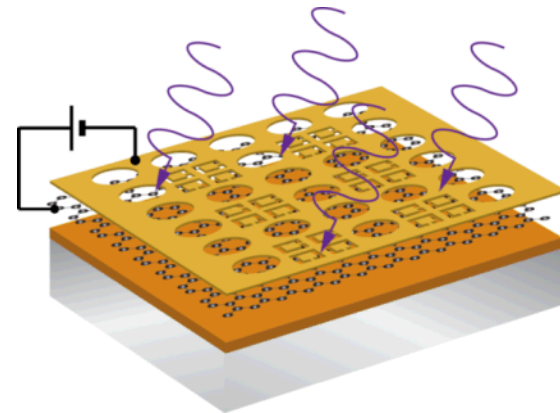
- Functionalized carbon nanotubes
- Giant quantum dots

Fabrication:

- Diamond centers
- Epitaxial quantum dots
- Meta-materials

Gaps

- Expanded ultrafast spectroscopy into new spectra
- New single photon sources
- Combing active and passive components into metamaterials
- Advanced nanofabrication and integration strategies for new materials systems and combinations of materials.



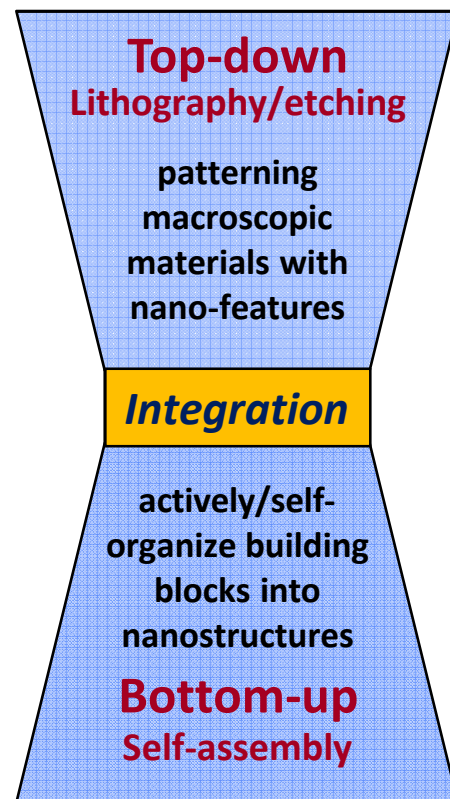
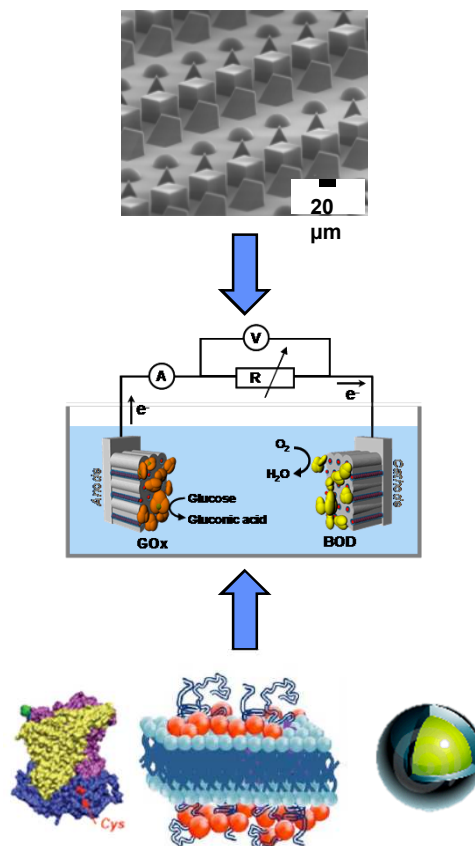


Hierarchical Soft Matter

Scientific opportunity: Propagate the intrinsically unique behaviors of nanoscale materials through novel strategies hierarchical assembly of functional materials.

World-leading science and capabilities:

- Synthesis of natural and engineered functional nano-constituents;
- Design, modification, and production of functional biomolecules;
- Modeling of the interactions and structures of soft materials.





Challenges

Integration:

- Achieve long-range order through understanding the interaction of the self-assembled structures with the macroscopic pattern.
- Reduce defects in self-assembled soft and composite nanomaterials.

Characterize:

- hierarchical assembly with improved spatial and temporal resolution
 - Enhance spatial and temporal characterizing through new multi-modal characterization tools

Modeling challenge:

- Developing multi-scale codes that predict the assembly behavior with relevant temporal and spatial scales.



Enabling Science through Capabilities

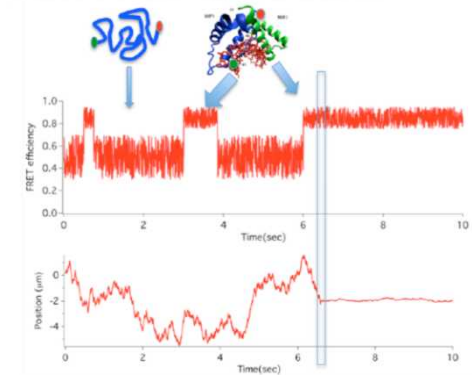
Near term:

- 2D and 3D soft fabrication - Top-down lithographical and patterning processes for novel platforms to control/guide spatial self-organization across multiple length scales and multiple dimensions
 - Micro-/nano-contact printing



Longer term:

- Characterization tools – develop new world-leading characterization tools to facilitate dynamic, multi-modal characterization:
 - X-ray diffraction w/ 3D optical tracking – Tools to concurrently measure ensemble averages and discrete components.
 - Lab in a Gap – Modified Discovery platform for direct observation of local hieratical assembly.
- Developing coarse-grain models with expanded spatial and temporal range.





New Capabilities Are Needed

To meet these nanomaterials integration challenges new generations of capabilities must be developed.

Internally by CINT



Host labs





Leverage Host Lab Facilities

National High Magnetic Field Laboratory



In-situ Ion Irradiation Transmission Electron Microscopy (I3TEM) – combined experiments in high temperature, flowing liquid, gas exposure, mechanical loading, displacement damage, gas implantation all in a TEM.

Laboratory for Ultrafast Materials and Optical Science (LUMOS) - understand and control the interaction of photons with materials' electronic, spin, and structural behavior on the ultrafast time scale.

Ion Beam Materials Laboratory - ion beam analysis techniques such as Rutherford backscattering spectrometry (RBS), nuclear reaction analysis (NRA), elastic recoil detection (ERD), particle-induced i- or gamma-ray emissions (PIXE or PIGE), and ion channeling.

MESA Micro Fab

Radiation hardened microelectronics as well as other advanced components such as micro-machines, optoelectronics, and photonic systems.





CINT's Future Capability – Short term

NEM

- **Single electron TEM camera Gatan K2 (\$550k)**
- Laser light source for PEEM (\$125k)
- \$250K, Keyence - 3D or other high end microscope as an addition, to compliment SEM.
- \$175K, Heidelberg - benchtop Direct Write Laser lithography tool to compliment the mask writer but for open access to the users.
- \$150K XActix - XeF2 Si etch reactor

NPON

- **NeaSPEc SNOM ~\$500k** – combined Near-field optical and AFM tool
- FTIR Microscope ~ \$100K
- ICP-OES system ~ \$90K
- Superconducting Nanowire Detector system ~\$140K
- Reggae laser repair ~ \$100K
- Actively controlled dye laser system ~ \$100K
- 3D Profilometer ~ \$120K

SBCN

- Raman spectroscopy (\$40K)
- Quartz crystal microbalance (\$60K)
- Akta pure protein chromatography system (\$70K)
- Liquid chromatography – mass spectrometry (IC-MS) (\$120K)
- Simultaneous, multi-color total internal reflectance fluorescence (TIRF) microscope (\$300K)
- ICP (\$110K)
- Magnetometer (\$120K)



CINT's Future Capability – Longer term

CINT's planned major new capabilities:

- **Soft lithography:** Top-down patterning / lithography combined with self-assembled (bottom-up) soft materials.
- **New Discovery Platforms** - Liquid-nanomechanics TEM Discovery Platform, new *in-situ* analysis techniques for the Microfluidic platform.
- **Quantum Materials Integration** – New atomic precision fabrication capabilities (p-dopant, III-V substrates), predictive qubit physics based models.



Take Home Points

- CINT is working on addressing the challenges to nanostructure integration.
- CINT is continually engaged with the community to determine high-impact nano-integration challenges.
- Working to provide the Science community with an evolving set of world-leading capabilities.
 - Some capabilities developed internally of CINT
 - Many leveraged from the host laboratories

CINT

The Center for Integrated Nanotechnologies

Nanomaterials

Integration

A U.S. DOE Nanoscale Science Research Center

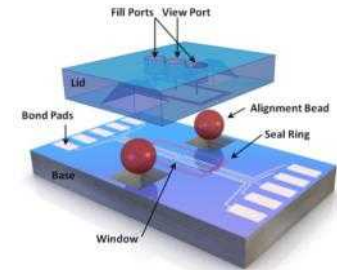
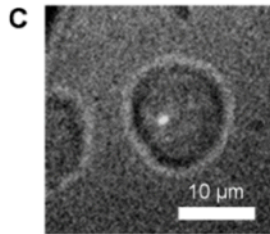
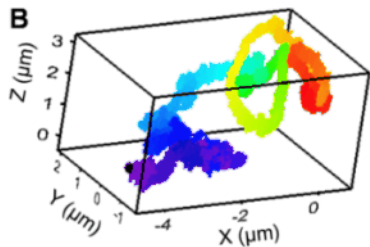
The CINT scientific community is enabling the Nation's future through excellence in research.





Capabilities to Address the Challenges

Tools: Offering world-leading equipment for the user community.



Scientists: Unique knowledge and skills to help CINT's users perform world-leading science.



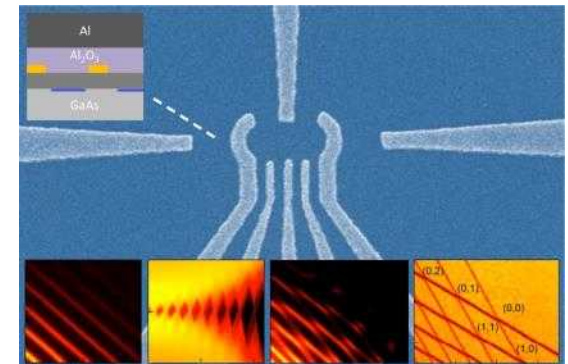
Quantum Materials Integration

To maximize CINT's impact on the user community we must continually look for opportunities.

Quantum materials has been identified by BES as an area of basic research need, which could impact energy technologies.[1]

CINT's Leadership

- Optical interactions with matter
- Low temperature transport in semiconductors
- Nano-fabrication and integration



[1] Feb. 2016 BES workshop on Basic Research Needs for Quantum Materials (<http://www.orau.gov/brnworkshop2016/charge.htm>)



Challenges – Recruitment & Retention

The Challenge – Maintaining Talent Pipeline

- *Career advancement opportunities (line and program management, retirement)*

Meeting the Challenge

- *Strong institutional reputations provide natural draw of new talent*
- *Continually evolve and update succession plans*



Challenges – Recapitalization

The Challenge – Science could be equipment-limited

- *Technique development and instrument acquisition are essential to user facility vitality*
- *Initial instrumentation set (circa 2006) is aging; cleanroom tools are a critical need*
- *Capital equipment costs (>\$500K) exceed discretionary funds available within operating budgets*

Meeting the Challenge

- *DOE mandated to spend 10% operating budget on recap.*
- *Leverage host-Lab, e.g.*
 - *LANL microscopy facility access*
 - *SNL and LANL high-performance computing capabilities*



Host Labs Support

Host Lab Capability Support:

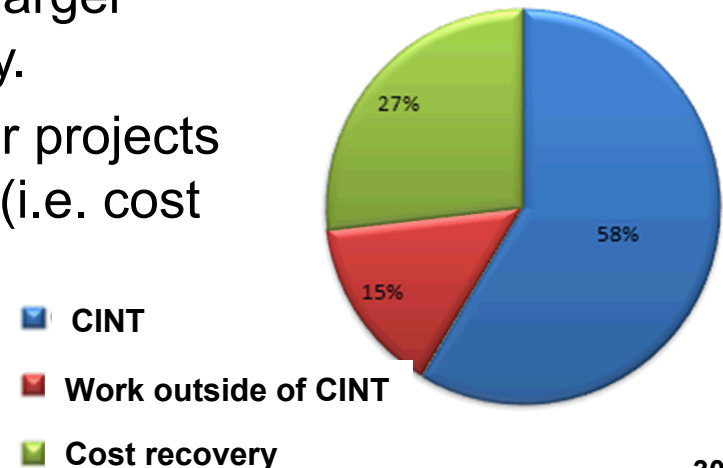
- Major investments in equipment at CINT
 - Gateway soft fabrication capability
 - Upgrades to the III-V MBE
- Lab funded access to high performance computing for User projects.
- LDRD and mission funded for capability development (e.g. Atomic Precision Fabrication)

Host Lab Support of Scientist Time:

- Host lab funding allows CINT to offer a larger verity of expertise for the User community.

~27% of the CINT Scientist's time on user projects is paid for by mission and LDRD funding (i.e. cost recovery).

Average Scientist time charging





Quantum Materials – Lab Investment



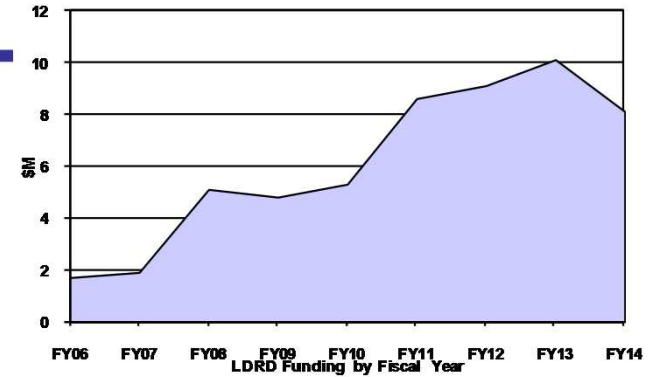
FY08 – FY10
Si-based qubits



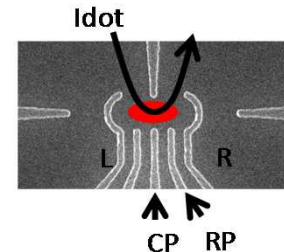
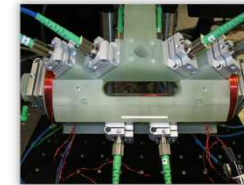
FY11-FY13
Architectures



FY14-FY16
Comms/QKD

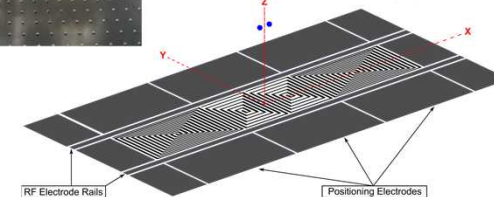
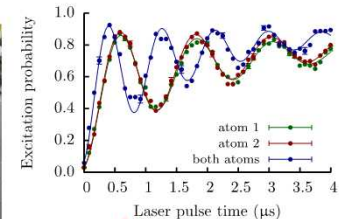
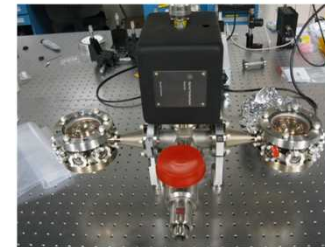


- Build foundational capabilities while exploring novel, high risk areas
- Focus on the engineering challenges of QIS
- \$62.6M investment, FY06-15
- Includes early career, traditional, and grand challenge LDRDs
- Essential vehicle for academic collaborations



• Broad and deep portfolio, spanning many facets of Quantum Materials:

- Qubits: physical qubit development, logical qubit design, entanglement, noise modeling
- Quantum engineering: architectures, robust controls for quantum gates, on-chip microwave control of ion traps, tomography
- Algorithms/applications: demonstration of few-qubit apps, algorithm design
- Simulation: design toolkits, error correction threshold simulators
- Sensing: matter-wave sensors, atom interferometry
- Comms: QKD, photon source development, single photon detectors



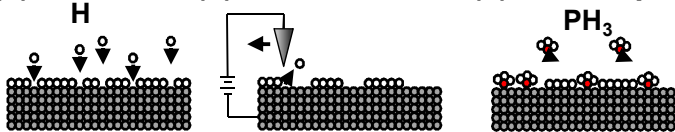


Atomic Precision Fabrication @ CINT

1st in US, only 1 at a user facility



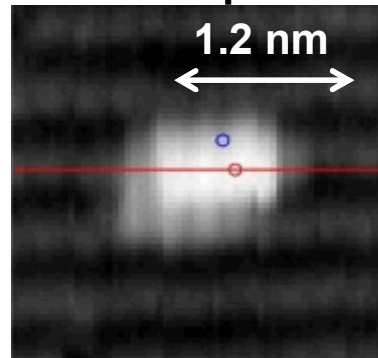
(1) Absorb H (2) Litho via STM (3) CVD doping



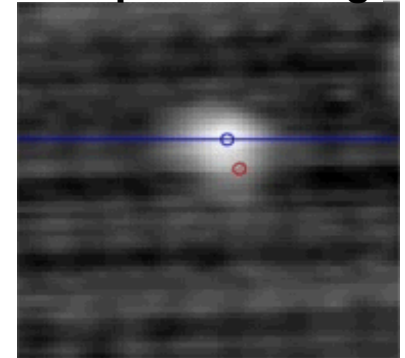
In-situ capabilities under development:

- Epitaxial growth capability for Si and ²⁸Si
- Delta doping of boron
- Ge and SiGe epitaxial growth

STM litho pattern



Incorporated single P



- E. Bussmann et al. Nanotechnology 26, 085701 (2015)
- W.C.T. Lee et al., Nanotechnology 25, 145302 (2014)

These capabilities can be accessed by users to explore defects and devices at the single atom level!



Qubit Physics Modeling

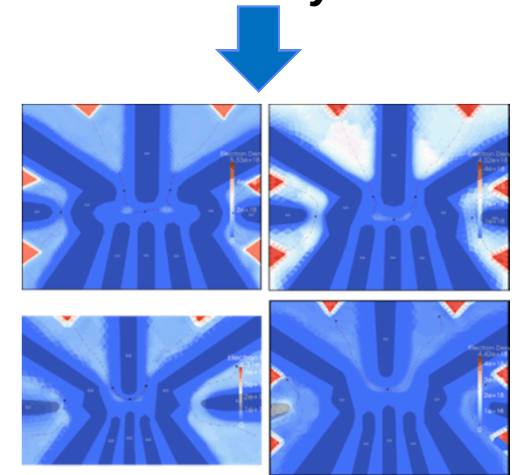
The QCAD model applies the, NNSA funded, Dakota solver to predict and evaluate the dynamic electrical performance of multi-dimensional quantum devices.

Uniqueness:

- The core contains nonlinear Poisson, effective mass Schrodinger, and Configuration Interaction solvers that have massively parallel capability for high simulation throughput, and can be run individually or combined self-consistently for 1D/2D/3D quantum devices;
- The core solvers show superior convergence even at near-zero-Kelvin temperatures, which is critical for modeling quantum computing devices;



QCAD model of Double Quantum Dot electron density



[Quantum computer aided design simulation and optimization of semiconductor quantum dots](#), X Gao, et al - Journal of Applied Physics, 2013

[The Promise of Quantum Simulation](#), RP Muller, et al - ACS nano, 2013

These capabilities could be accessed by CINT users to model and understand their integrated quantum devices (qubit).