Research at Los Alamos National Laboratory

Theme 3: Materials and Chemical Research

Andrew Dattelbaum
Division Leader
Materials Physics and Applications

Dec. 3, 2021

Long-term ST&E stewardship is based on Capability Pillars

- Our capability pillars define six key areas of science, technology, and engineering in which we must lead

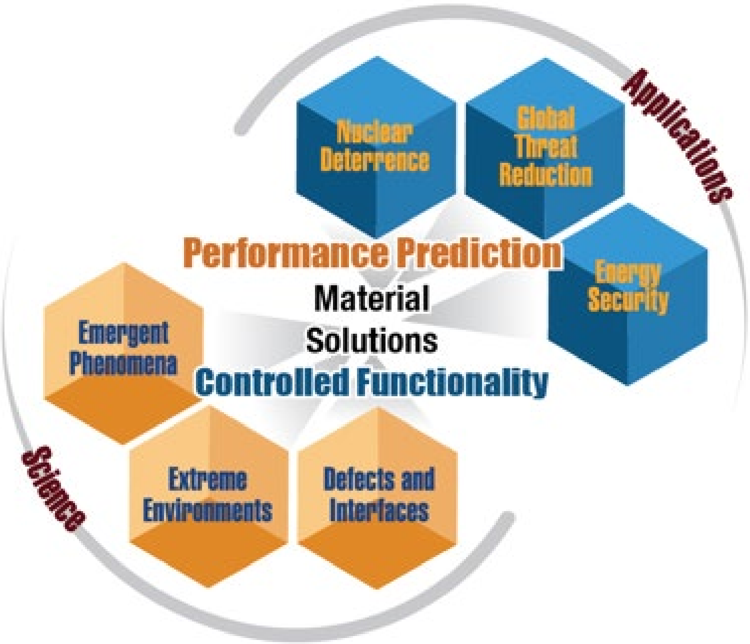
Engineering	MATERIALS FOR THE FUTURE	Defects and Interfaces Extreme Environments Emergent Phenomena
	NUCLEAR AND PARTICLE FUTURES	Applied Nuclear Science & Engineering Nuclear & Particle Physics, Astrophysics & Cosmology Accelerator Science & Technology High Energy Density Physics & Fluid Dynamics
	INTEGRATING INFORMATION, SCIENCE, AND TECHNOLOGY FOR PREDICTION	Computing Platforms Computational Methods Data Science
	SCIENCE OF SIGNATURES	Nuclear Detonation Nuclear Processing, Movement, Weaponization Natural and Anthropogenic Phenomena
	COMPLEX NATURAL AND ENGINEERED SYSTEMS	Human–Natural System Interactions: Nuclear Engineered Systems Human–Natural System Interactions: Non-Nuclear
	WEAPONS SYSTEMS	Design Manufacturing Analysis

Materials Strategy Vision: Develop materials with controlled functionality and predictable performance

Vision
Controlled Functionality and
Performance Prediction

Strategy
We predict performance and control functionality through forefront science and engineering across three themes:

- Defects and Interfaces
- Extreme Environments
- Emergent Phenomena



Execution
Strong coupling between experiment, theory, modeling and simulations

Materials for the Future Strategy links leadership areas through science themes to achieve overarching goals

GOALS						
Performance Prediction and Controlled Functionality						
SCIENCE THEMES						
Defects and Interfaces						
Extreme Environments						
Emergent Phenomena						
AREAS OF LEADERSHIP						
Complex Functional Materials	Material Resilience in Harsh Service Conditions	Manu-facturing Science	Actinides & Correlated Electron Materials	Integrated Nano-materials	Energetic Materials	Materials Dynamics

Los Alamos NATIONAL LABORATORY

Vision and Mission Statements for the Materials Physics and Applications Division

Vision Statement

MPA, as LANL's flagship experimental fundamental science organization, is sought out across LANL as the premier partner for solving the world's most difficult scientific problems.

Mission Statement

We conduct world-class research in materials science and enable the development of new technologies that solve pressing national energy and security challenges by:

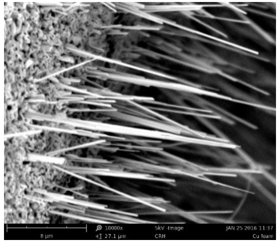
- discovering materials and exploring their properties,
- developing new characterization tools and practical applications of materials,
- understanding and exploiting quantum phenomena, and
- providing world-class user facilities.

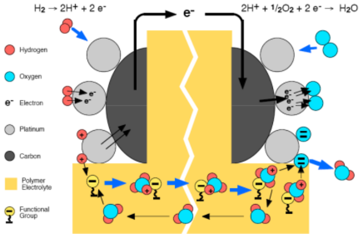
Materials Synthesis and Integrated Devices (MPA-11): An Applied Energy Group

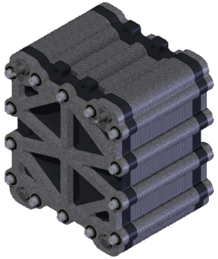
- Our mission is to provide innovative and creative chemical synthesis and materials science solutions to solve materials problems across the broad LANL missions.

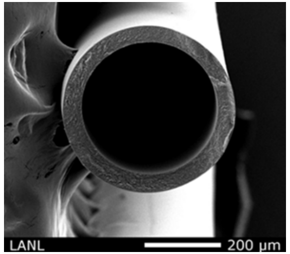
- Our group conducts basic and applied research in areas related to Energy Security as well as problems relevant to the Weapons Program.

- Polymer Electrolyte Fuel Cells
- Acoustic Sensors
- Advanced Separations
- Polymer membranes for gas separations
- Nanomaterials synthesis of 2D materials
- Electrochemical-based gas sensors and devices





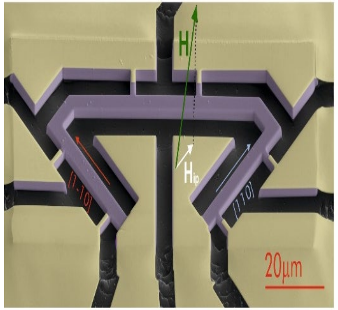


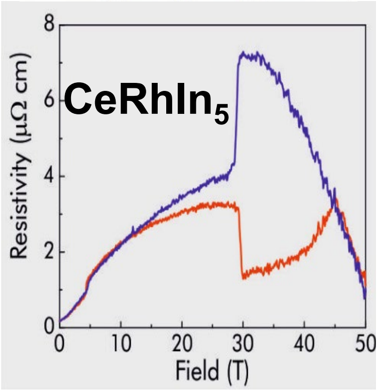


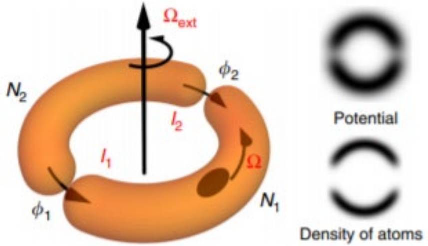
The Quantum group (MPA-Q) focuses on quantum-based research and development

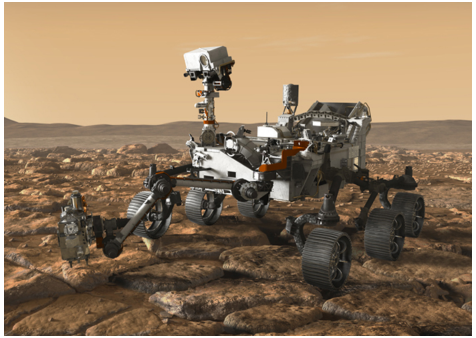
Focus Areas:

- Magnetic Sensing and Miniaturization
- Quantum Communication Systems
- Quantum and Strongly Correlated Electron Materials
- Quantum Technologies





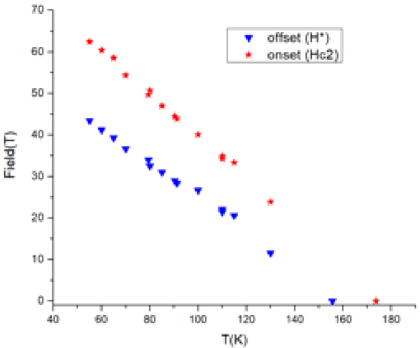




MPA-MAGLAB: The Magnet Lab Pulsed Field Facility is Part of the National High Magnetic Field Laboratory

- **Operate a world-leading high-magnetic-field user program**
- **Carry out in-house research in support of the user program**
- **Maintain facilities and develop new magnets/instrumentation**
- **Conduct education and outreach activities**

75T duplex magnet installation



H_3S superconductor measured at 170 GPa in 65T pulsed magnet

100 T pulsed fields

Primary Sponsor:

NSF

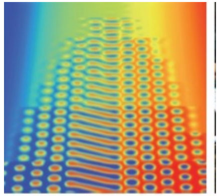
Partnership with:

FLORIDA STATE UNIVERSITY

UF UNIVERSITY of FLORIDA

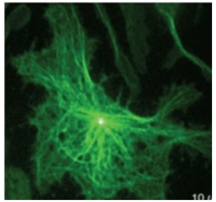
Los Alamos NATIONAL LABORATORY

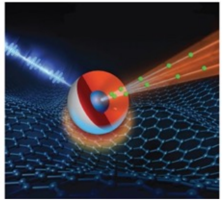
The Center for Integrated Nanotechnologies (MPA-CINT)



<u>Scientific Thrusts</u>

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



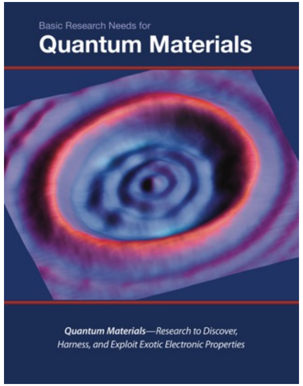


DOE-Funded Nanoscience User Facility

The CINT user program provides access to nanoscale synthesis, characterization and theory to BES-MSE programs

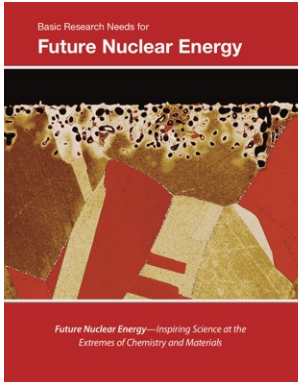
LANL BES Materials Strategy Builds Upon Established Leadership in Key Research Areas at LANL

- **Correlated Electron Materials with a focus on Quantum Matter**
- Leveraging LANL's strengths in Actinides and Correlated Electron Materials, as well as Integrated Nanomaterials, grow our world-leading BES program in Experimental & Theoretical Condensed Matter Physics.



- **Mechanical Behavior and Radiation Effects**

Leveraging LANL's strengths in Materials Dynamics and Materials Resilience in Harsh Conditions, grow our world-leading BES program in Mechanical Behavior and Radiation Effects spanning atomistic to the nanoscale to the mesoscale.



LANL has a Multi-faceted Quantum Strategy that is Synergistic with Office of Science Programs

- Science Frontiers
- "Co-Design"

ASCR	BES	HEP	NP
Quantum algorithms; uncertainty quantification and verification & validation methods; software stack; quantum networks	Synthesis, characterization, theory, modeling, and instrumentation to advance quantum materials & chemical phenomena	Black hole physics; quantum gravity and quantum error correction; fundamental aspects of entanglement	Isotopes and trapped ions for quantum devices; lattice quantum chromodynamics

Quantum Field Theory and Topology

Control of Quantum Phenomena

SC

HEP, NP: Theory, physics, detectors
BES: Matls ➔quantum; quantum ➔matls
BER: Quantum Imaging
ASCR: Quantum algorithms & testbeds

Center for Integrated Nanotechnologies (CINT)

QUANTUM SCIENCE CENTER

Advanced Simulation & Computing

Strategic Partnerships

NNSA Mission Needs

Institutional Investment
- Competitive LDRD; Early Career Awards
- Rapid Response Efforts; Summer Schools

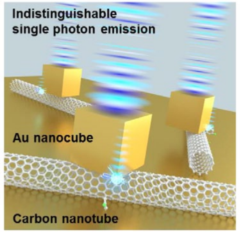
QuAInT: Quantum Accelerated Internet Testbed

Objective: Advance the high-priority research directions and milestones identified in the DOE Quantum Internet Blueprint Workshop report.

PI: Nicholas A. Peters, ORNL

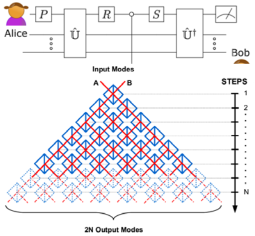
Deputy-PI: Raymond Newell, LANL

Quantum Emitter Single Photon Sources



Satellite Design requirements analysis

Quantum Information Scrambling



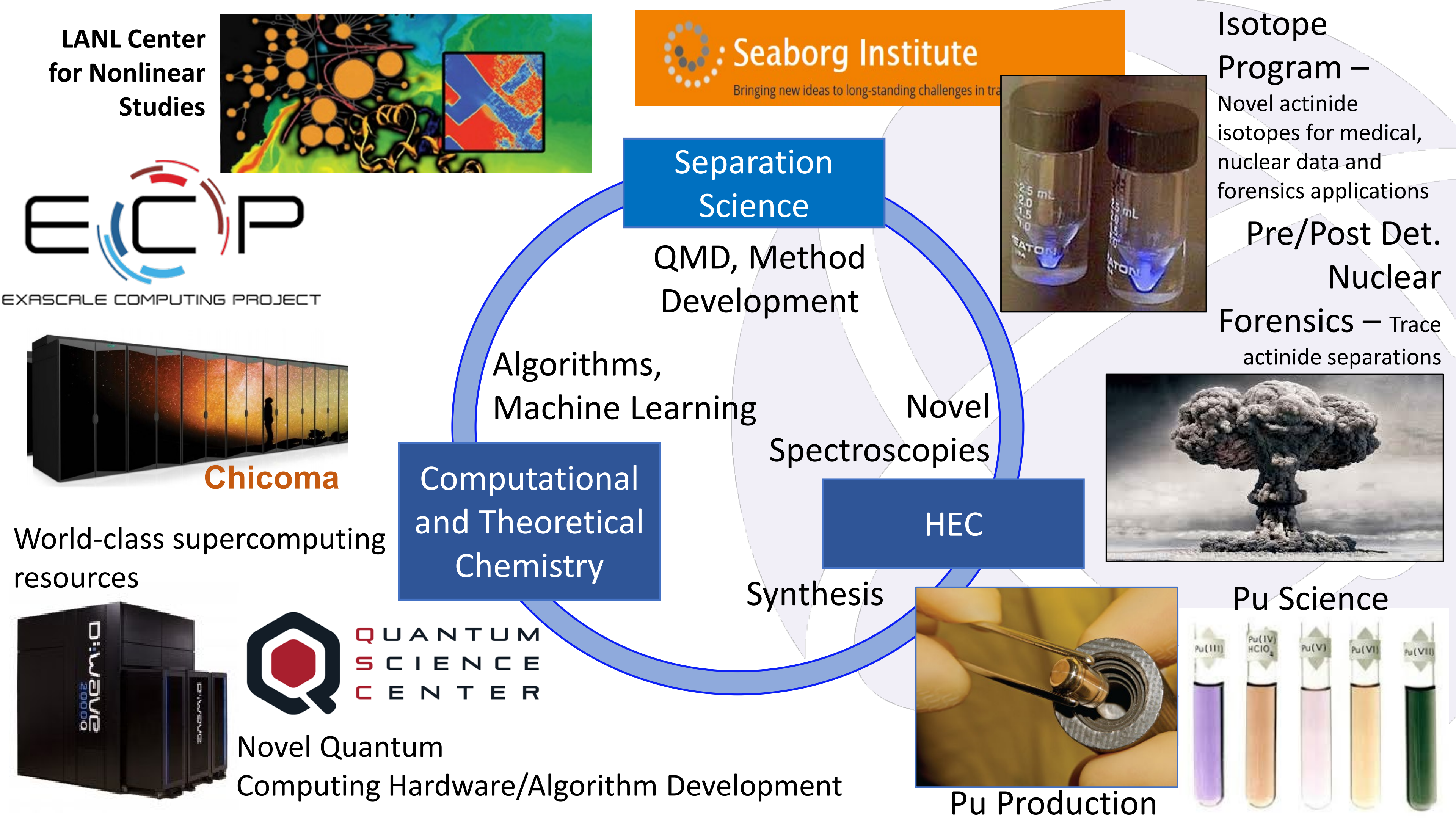
Approach:

Design, develop, and demonstrate a regional-scale intracity quantum internet testbed along with the required components, subsystems, and control systems.

Key technologies include single and entangled photon sources, quantum memory, and quantum processing on frequency modes.

Partners

Los Alamos National Laboratory · Oak Ridge National Laboratory · Purdue University · The University of Tennessee Knoxville · Qubitekk · aws


LANL Center for Nonlinear Studies
Seaborg Institute
Bringing new ideas to long-standing challenges in tra
Isotope Program –
Novel actinide isotopes for medical, nuclear data and forensics applications
ECP
EXASCALE COMPUTING PROJECT
Separation Science
QMD, Method Development
Pre/Post Det. Nuclear Forensics – Trace actinide separations
Chicoma
Algorithms, Machine Learning
Novel Spectroscopies
Computational and Theoretical Chemistry
HEC
World-class supercomputing resources
Synthesis
Pu Science
Pu(III)
Pu(IV) HClO4
Pu(V)
Pu(VI)
Pu(VII)
QUANTUM SCIENCE CENTER
Novel Quantum Computing Hardware/Algorithm Development
Pu Production

BACK UP SLIDES

LANL is a core partner in the Quantum Science Center (QSC) Led by ORNL

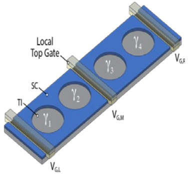
QUANTUM SCIENCE CENTER

QSC mission: Integrate the discovery, design, and demonstration of revolutionary topological quantum materials, algorithms, and sensors catalyzing development of disruptive technologies.

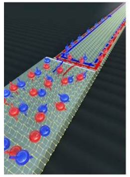
QSC scientific goals are to:

- Design topological materials that do not degrade quantum information
- Create and implement algorithms that exploit topological systems
- Design and deploy novel quantum sensors that make the unmeasurable measurable

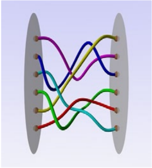
2D Quantum Materials



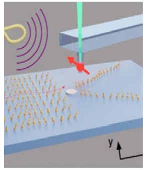
Edge States



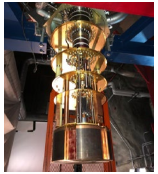
Interacting Systems (Anyon Braiding)



Prototype Sensors



Deployable Devices

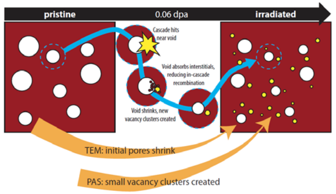


Fundamental Science → Devices → Prototypes → Applications

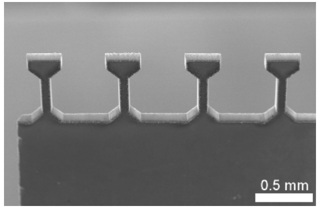
Los Alamos National Laboratory | Oak Ridge National Laboratory | Fermilab | Microsoft

Material Resilience in Harsh Service Conditions integrates AoLs through combined, extreme environments

- Capability to measure, predict, and control the nature and evolution of properties to allow building in resilience is crucial to national nuclear, global, and energy security missions



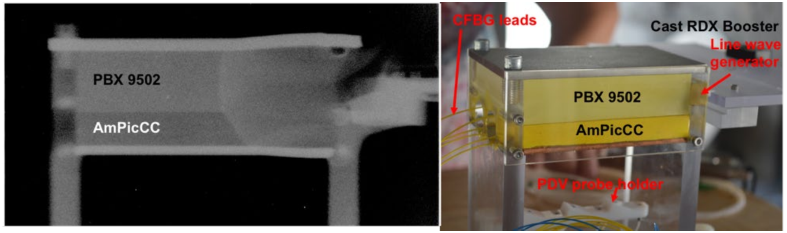
Irradiation/corrosion studies



Microscale mechanical testing

Energetic Materials AoL focuses on safe and predictable performance

- Design high energy metastable molecules, engineer composite formulations and process parameters that link to safety and performance characteristics
- Stockpile needs require both experiments and modeling to develop microstructural awareness in energetic materials

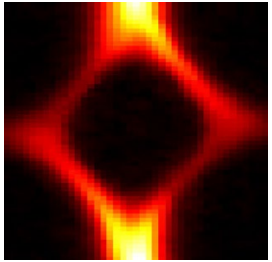


Novel HE formulations and dynamic experiments validate models to predict performance

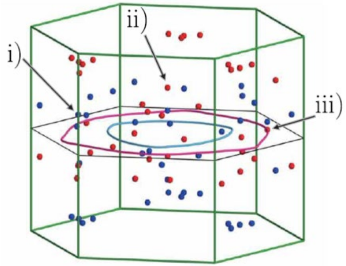
Los Alamos NATIONAL LABORATORY

Actinides and Correlated Electron Materials ties foundational research to mission needs

- Understanding and controlling emergent electronic states
- Predictive performance of actinide materials



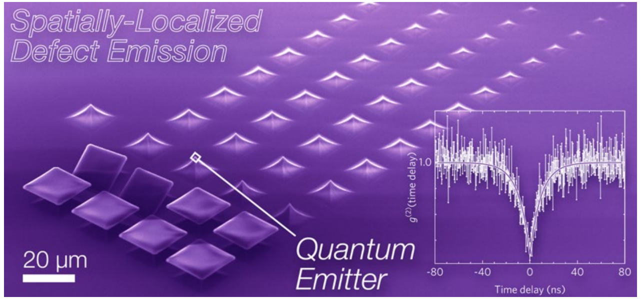
Noise measurements of magnetic monopoles in spin ice (PRX 2021)



Colossal thermoelectric response in a uranium ferromagnet (Sci. Adv. 2021)

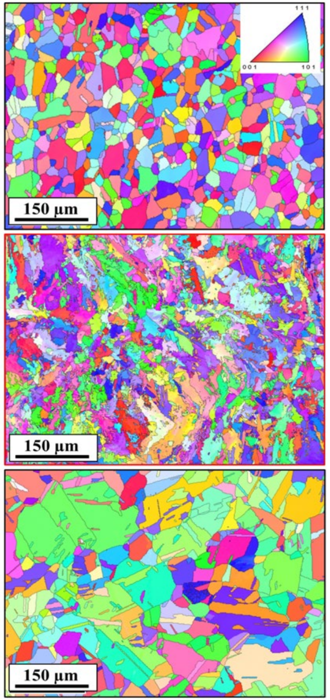
Integrated Nanomaterials goes beyond nano-building blocks

- Define and control nanomaterials organization, interaction, and interfaces across length scales as key to accessing and controlling functionality
- Integration as an enabler to discovery and use of emergent properties

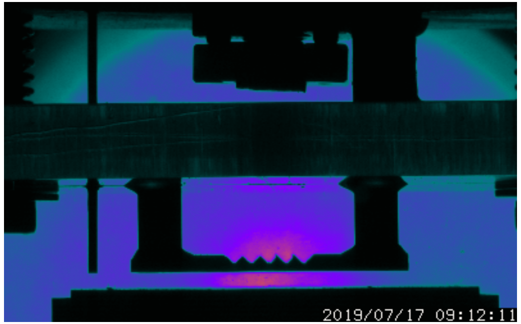


Materials Dynamics focuses on microstructure-aware performance at high strain rates and pressures

- Understanding process-structure-properties-performance (PSPP) is increasingly important for manufacturing efficiencies, new material qualification, agility, etc.
- Realization of advanced models for PSPP for more predictive behavior requires data science to address big data sets - especially from light sources; focus on AI/ML for models
- Increased focus on need for scale bridging (“meso” to continuum)
- Diagnostics and new tests – need better characterization of sample pedigree, and more sensitive tests to address physics
- Using and advancing existing light sources



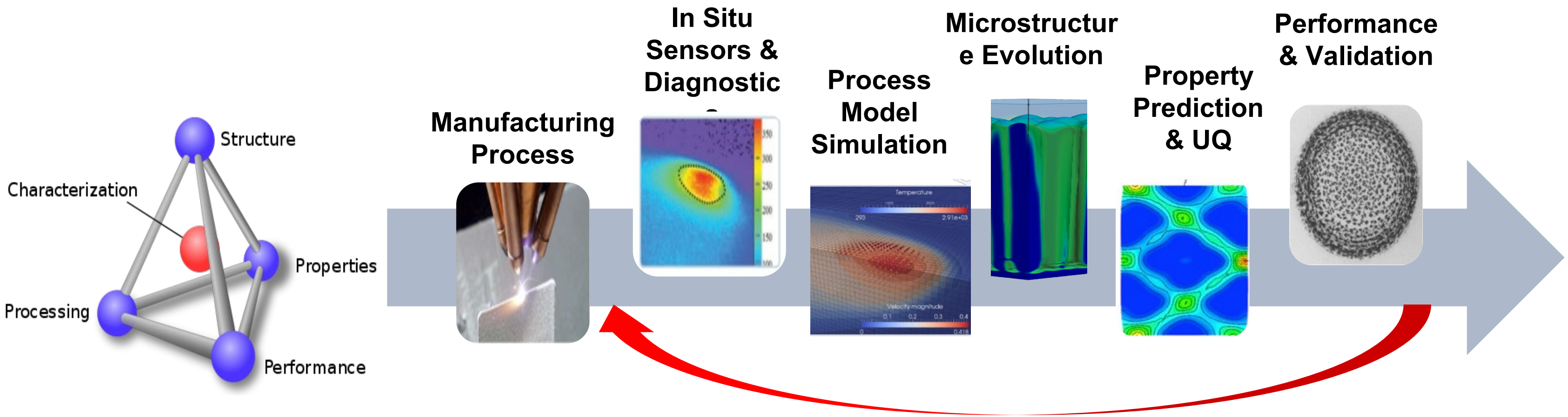
100 and 80 mm guns in MST-8



Complex Functional Materials **integrates across AoLs**

- Comprised of multiple components or building blocks that are integrated or chemically bound together to achieve a desired function or response
- Emphasis on soft materials and structural properties at the meso- and micro-scale that control materials function
- Must satisfy multiple criteria essential to the overall application such as materials for:
  - Responsive stockpile: structural components and "aware materials"
  - Energy conversion and energy storage: CFM that enable net-zero CO_2 energy
  - Sensors and detectors: chemical, biological, radiological, nuclear, and explosives sensors and detection
  - Computing and communications

Manufacturing Science spans both small scale science, as well as the LANL Production Mission



- Strategically invest to enable successful manufacturing pathway development through:
  - Enabling agile programmatic manufacturing response and maturation of new manufacturing capabilities
  - Coordinating development of experimental, modeling, and information science tools to manufacture materials with controlled functionality and predictable performance
  - Coupling an in-depth materials, process knowledge with appropriate *in situ* monitoring, *ex situ* inspection, and predictive simulations to allow for a flexible and agile manufacturing capability

The Materials Pillar supports several national user facilities and utilizes facilities at other institutions

CINT:
Nanomaterials synthesis and characterization

Materials-centric national user facilities

NHMFL-PFF:
Research with high magnetic fields

LANSCE
Los Alamos Neutron Science Center

Research with protons and neutrons

LCLS

Advanced Photon Source

SNS
SPALLATION NEUTRON SOURCE

The LANSCE facility has a diverse set of capabilities—many are essential for the Materials Pillar

- **Operations began in 1972**
  - Risk mitigation project completed in 2015; other efforts underway for sustainability
- **800-MeV (1 MW) proton beam**
- **Highly capable/flexible facility**
  - 100-800 MeV proton energies
  - 6 target stations
  - 3 neutron spallation targets
  - 16 beam lines
  - Time structure of beam allows for a large dynamic range of experiments
- **Dynamic proton radiography**
- **Neutron radiography**
- **Structural material properties**
- **Nuclear properties of materials**
- **Fundamental physics**
- **Isotope production**