Research at Los Alamos National Laboratory

Theme 3: Materials and Chemical Research

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Materials Physics and Applications
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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

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<th>Integrating Information, Science, and Technology for Prediction</th>
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<th>Complex Natural and Engineered Systems</th>
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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

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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.

• 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

Primary Sponsor:

H$_3$S superconductor measured at 170 GPa in 65T pulsed magnet

100 T pulsed fields

Partnership with:

75T duplex magnet installation
The Center for Integrated Nanotechnologies (MPA-CINT)

Scientific Thrusts
- 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”

**ASCN**
- Quantum algorithms; uncertainty quantification and verification & validation methods; software stacks; quantum networking

**BES**
- Synthesis, characterization, theory, modeling, and instrumentation to advance quantum materials & chemical phenomena

**HEP**
- Black hole physics; quantum gravity and quantum error correction; fundamental aspects of entanglement

**NP**
- Isotopes and trapped ions for quantum devices; lattice quantum chromodynamics

- HEP, NP: Theory, physics, detectors
- BES: Matls \(\rightarrow\) quantum; quantum \(\rightarrow\) matls
- BER: Quantum Imaging
- ASCN: Quantum algorithms & testbeds

**Advanced Simulation & Computing**

**Strategic Partnerships**

**Institutional Investment**
- Competitive LDRD; Early Career Awards
- Rapid Response Efforts; Summer Schools
QuAlInT: Quantum Accelerated Internet Testbed

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

*Pl: Nicholas A. Peters, ORNL*

*Deputy-PI: Raymond Newell, LANL*

**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.
**Seaborg Institute**

Bringing new ideas to long-standing challenges in trans-fusion science.

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**LANL Center for Nonlinear Studies**

- **QMD, Method Development**
- **Synthesis**
- **Algorithms, Machine Learning**
- **Novel Spectroscopies**
- **HEC**

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**ECP** (Exascale Computing Project)

- Chicoma
- World-class supercomputing resources

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**Quantum Science Center**

- Novel Quantum Computing Hardware/Algorithm Development

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**Pu Science**

- Pu Production
- Isotope Program – Novel actinide isotopes for medical, nuclear data and forensics applications
- Pre/Post Det. Nuclear Forensics – Trace actinide separations

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**Pu Science**

- Novel Quantum Computing Hardware/Algorithm Development
BACK UP SLIDES
LANL is a core partner in the Quantum Science Center (QSC) Led by ORNL

**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**
**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

**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

Irradiation/corrosion studies

Microscale mechanical testing

Novel HE formulations and dynamic experiments validate models to predict performance
Actinides and Correlated Electron Materials ties foundational research to mission needs

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

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
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 CO₂ 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 \textit{in situ} monitoring, \textit{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

Research with protons and neutrons
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