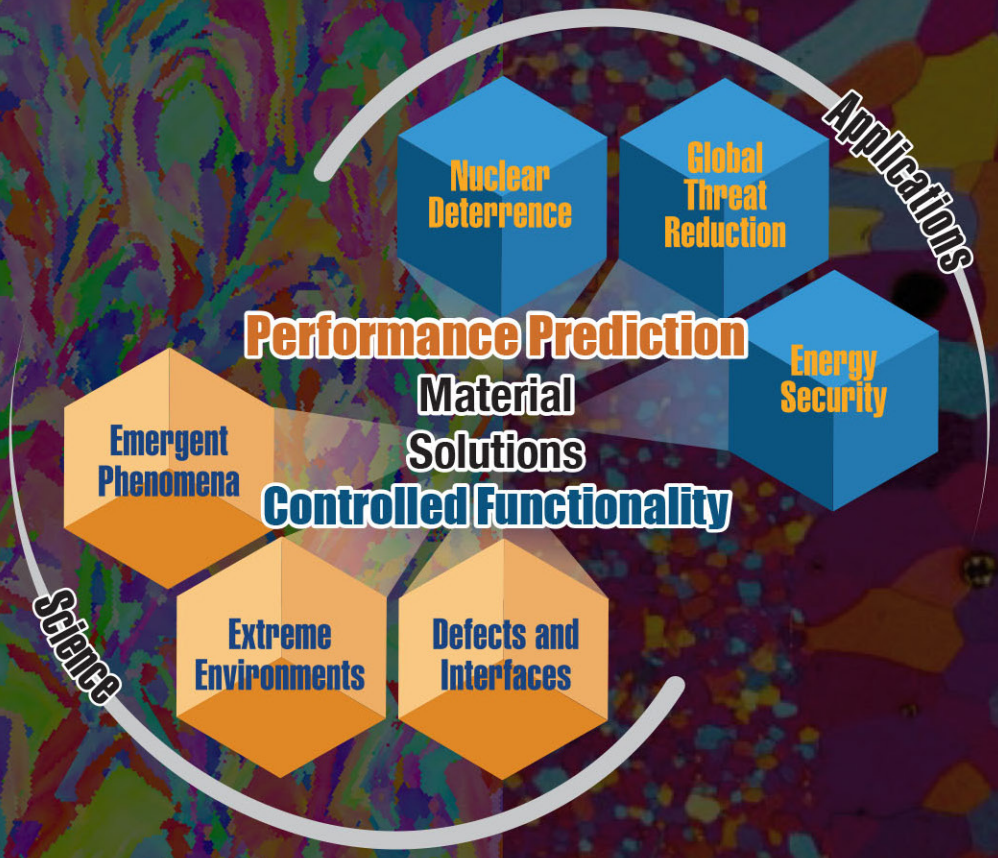
MATERIALS FOR THE FUTURE



Los Alamos
NATIONAL LABORATORY
EST. 1943

Solving national security challenges for nuclear deterrence,
global threat reduction, and energy security—
through controlled functionality of materials with predictable performance.

Meeting national security needs now and in the future

Los Alamos National Laboratory's mission is to solve national security challenges through scientific excellence. The Materials for the Future strategy is driven by our national security priorities of nuclear deterrence, energy security, and global security.

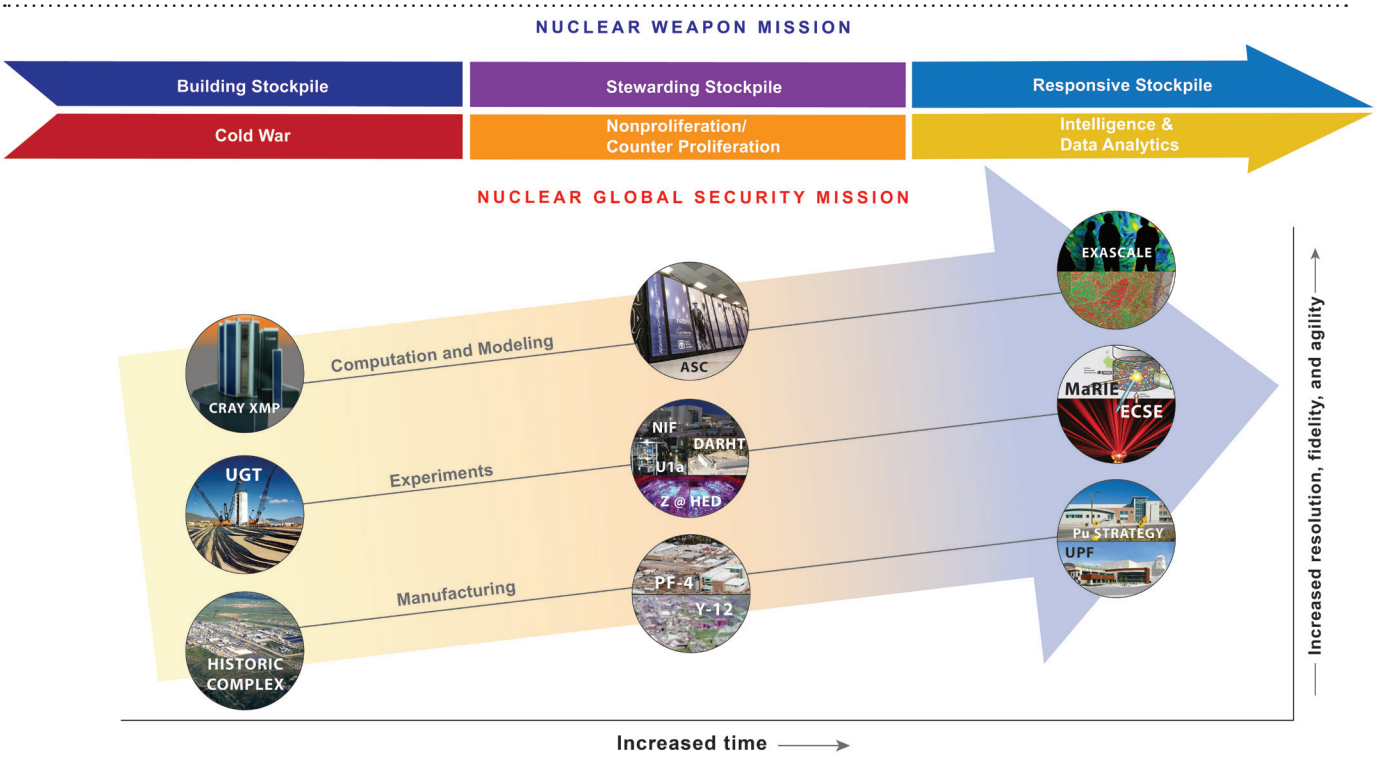
The overarching goal of our strategy is to support our mission by providing materials with controlled functionality and predictable performance with the agility to respond to ongoing and emerging mission needs. Fulfillment of our strategy supports meeting today's deliverables while preparing for tomorrow's challenges.

The National Landscape

Los Alamos National Laboratory executes work in all of the Department of Energy's (DOE) missions: national security, science, energy, and environmental management. Our contributions are part of what makes DOE a science, technology, and engineering powerhouse for the nation.

We focus on integrating research and development solutions to achieve the maximum impact on strategic national security priorities. In addition, through our partnerships across government agencies, laboratories, universities, and industry, we deliver the best possible science and technology results for the nation.

In 2014, Los Alamos National Laboratory published *Proud Legacy, Bold Future* to codify our scientific strategy. That document describes our core mission areas and the four science pillars that underpin our service to the nation.



As the nation has moved from building the stockpile to supporting a responsive stockpile, it requires tools, facilities, and expertise with increased resolution, fidelity, and agility. Our materials strategy, coupled with future experimental facilities, positions Los Alamos to meet these evolving mission needs. The illustration above provides the strategic context for our vision.

We

- provide a safe, secure, and effective stockpile;
- protect against the nuclear threat;
- counter emerging threats; and
- provide solutions to strengthen energy security.

These missions require a robust and flexible science base that we manage and develop using our science pillars, which are

- Materials for the Future;
- Science of Signatures;
- Nuclear and Particle Futures; and
- Integrating Information, Science, and Technology for Prediction.

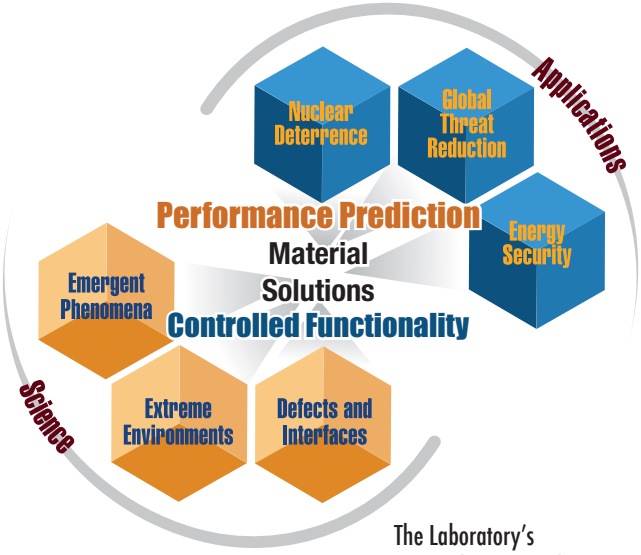
The pillar concept is the primary tool the Laboratory uses to plan for how we will accomplish both current and future missions.

Materials for the Future Capability

We pursue the discovery science and engineering for advanced and new materials to intentionally control functionality and predict performance to enable our missions.

We have updated our analysis of the forecasted materials science needs for our national security customers. Our assessment of these needs guides our overall strategy, identifying areas of leadership in which we must excel to successfully meet our mission objectives. Our areas of leadership are connected through common science themes. A key component of the materials strategy at Los Alamos is managing the capability to be agile for future national security needs in nuclear deterrence, energy security, and global security missions.

Delivering on our missions requires forefront science, technology development, and engineering that complement one another and build upon our established scientific strengths and innovative workforce. The materials capability will enable the achievement of the Laboratory's applications goals and, in turn, the Laboratory's mission needs will drive advancement of our science capability. The results will provide essential solutions to national security challenges, as conceptualized in the materials strategy diagram.



The Laboratory's materials strategy diagram.

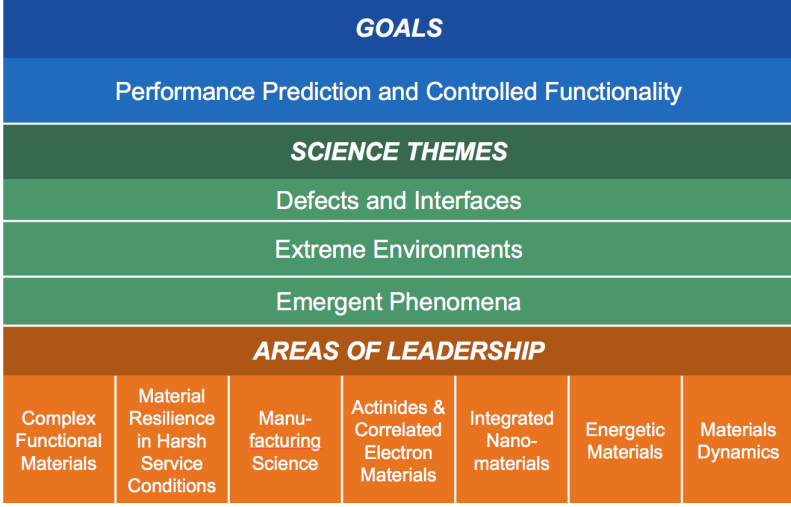
A key objective is to anticipate a mission need for specific materials performance and to position materials research to meet that need, which requires us to predict performance and control functionality in materials. Performance is the traditional terminology to describe how a material fulfills defined requirements. Prediction of a material's performance over its lifetime in a complex service environment is critical for accelerating new materials into applications. We use the term **predictable performance** to describe our ability to reliably and consistently forecast how a material will perform over its lifetime. We use the term **controlled functionality** to describe the actual design and tailoring of a material's properties that were previously unattainable or not available with traditional techniques. **Controlled functionality** and **performance prediction** are the core vision of our strategy.

Our overarching strategy in the Materials for the Future pillar is best represented by a matrix, where our **areas of leadership** are the columns of technical expertise that are needed for Los Alamos National Laboratory to successfully execute its materials strategy. The columns of leadership

areas are inter- and cross-connected by the three **science themes**, namely Defects and Interfaces, Emergent Phenomena, and Extreme Environments. The degree of penetration and interconnectedness by all three science themes varies for each area of leadership and allows for areas of synergy that provide fertile ground for interdisciplinary collaboration. Underlying this matrix and weaving all elements into an interconnected fabric is science at the mesoscale. Mesoscale is not only understood as a spatial dimension bridging the nano- and macroscopic scales, but as a multidimensional space that is characterized by the complexity of its phenomena at the transition from the discrete quantum to the continuum macroscopic world. Exploration of the mesoscale requires new tools and diagnostics and is driving the Laboratory's goal to build the new facilities MaRIE (Matter-Radiation Interactions in Extremes) and ECSE (Enhanced Capability for Subcritical Experiments).

Materials for Mission Needs

In supporting nuclear deterrence, we recognize that even today's stockpile is not static due to aging, manufacturing changes, material replacement, and the possibility for new mission objectives. Success with our materials strategy relies on the principle of co-design—or the close coupling between experiment, theory, modeling, and simulation.



Energy security can only be achieved with a focus on domestically produced energy, including the entire portfolio of oil and gas exploration, renewable sources, and nuclear energy. Materials needs arise from varying sources of energy with specific materials challenges, such as radiation-resistant cladding for nuclear fuel rods or advanced electrochemical systems for fuel cells and flow batteries. For all these systems, energy efficiency is a driving force to demand innovative material solutions.

Strategic deterrence and nonproliferation are key components of our global security mission. Materials needs arise in agile space applications with a

Science Pillars

The greatest science breakthroughs come from approaching difficult problems in revolutionary and interdisciplinary ways. Los Alamos National Laboratory's national security missions require an effective, flexible, forward-looking multidisciplinary approach to solve some of the nation's toughest science and engineering challenges.

Our flexibility comes from four key capability areas or "science pillars" that are fundamental to our missions. These pillars are sustained by our scientific expertise and our unique experimental and computational facilities. These same strengths also define our role in broader security missions and allow us to approach difficult problems in a new fashion and face national challenges we cannot yet imagine.

These science pillars are interlinked and build on the common foundation of seven decades of sophisticated discovery science that have been critical in ensuring national security.

- The Materials for the Future pillar optimizes materials for national security applications by predicting their performance and controlling their functionality through discovery science and engineering.
- The Science of Signatures pillar applies science and technology to intransigent problems of system identification and characterization in areas of global security, nuclear defense, energy, and health.
- The Nuclear and Particle Futures pillar integrates nuclear experiments, theory, and simulation to understand and engineer complex nuclear phenomena.
- The Integrating Information, Science, and Technology for Prediction pillar leverages advances in theory, algorithms, and the exponential growth of high-performance computing to accelerate the integrative and predictive capability of the scientific method.

focus on light-weighting and radiation resistance and in the dominance of the electromagnetic spectrum to ensure secure communication paths between ground-based and space-based terminals. There is a need to develop efficient and rapid response sensor and detector materials to capture and interpret signatures from multiple inputs, including electromagnetic, chemical, or biological sources.

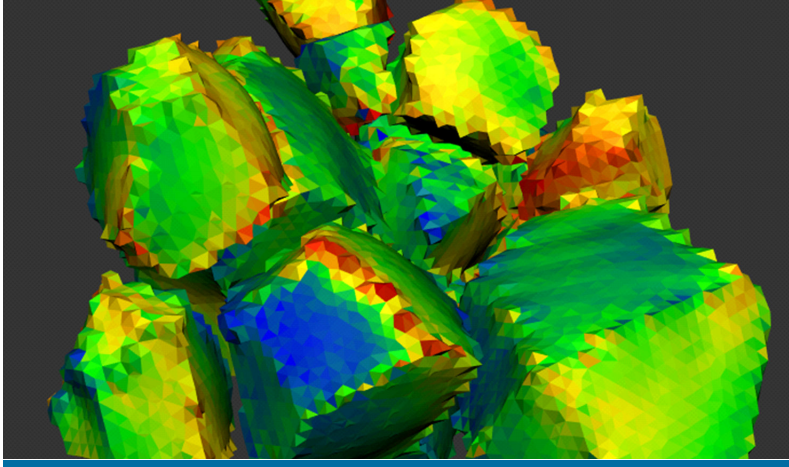
Science Themes

We strive to achieve controllable functionality and predictable performance even in extreme environments by manipulating defects and interfaces and through the deliberate introduction of emergent phenomena.

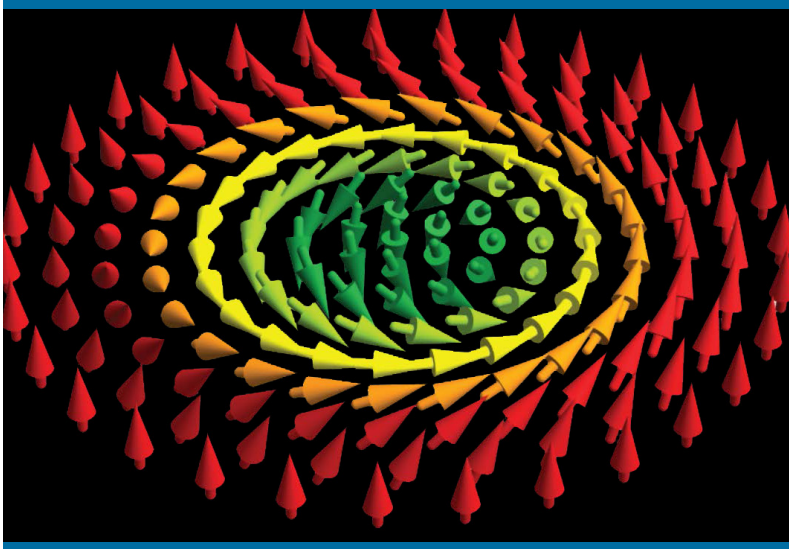
Defects and associated interfaces in otherwise homogeneous materials often dominate the material properties and can be exploited to design materials with new functionality. Novel manufacturing techniques that allow for atomic-scale manipulation and new characterization techniques at multiple length and time scales, including capabilities at the nation's light sources, combined with next-generation computational tools set the stage to control defects and interfaces to our advantage.

A similar revolution is taking place in the area of emergent phenomena—new collective behaviors that extend beyond the material behavior of each component. Emergent phenomena manifest themselves whenever we have multiple degrees of freedom in electron charge, spin, orbital, and lattice that interact in unexpected ways. Emergent behavior in materials is ubiquitous—including superconductivity, topologically protected states such as in vortices and skyrmions, and quantum entanglement.

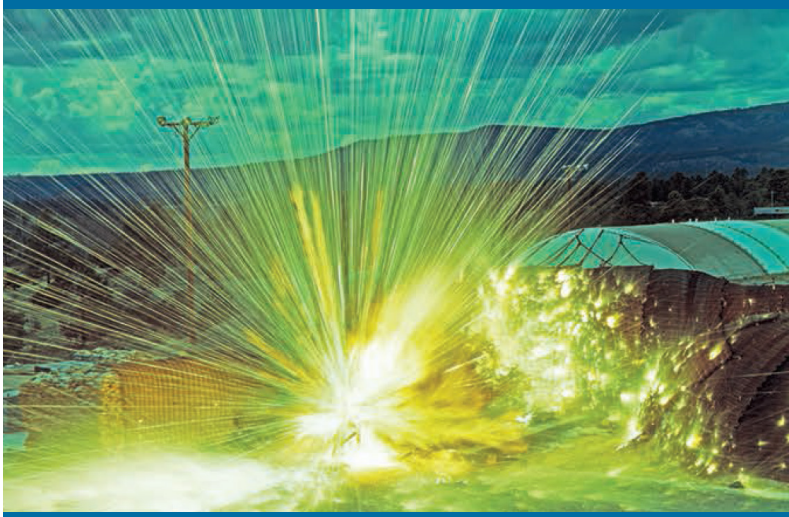
The study of a material's response to an extreme environment and its deliberate design to withstand this environment's effects is a central theme of our strategy given the Laboratory's mission. Two key factors need to be considered in this context: 1) the duration of exposure may convert



Defects and Interfaces: The mechanistic understanding and control of inhomogeneities, intrinsic and engineered, across all appropriate length and time scales that govern materials functionality.



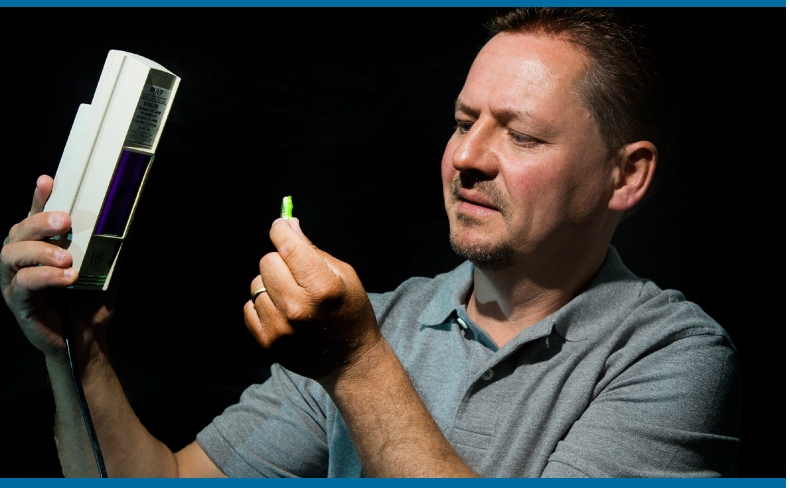
Emergent Phenomena: Complex and collective forms of matter that exhibit novel properties and respond in new ways to environmental conditions, enabling the creation of materials with innate functionality.



Extreme Environments: The underlying principles enabling the understanding of the interactions of materials with extreme conditions in order to create environmentally tolerant properties and the ability to exploit extreme environments to tune materials functionality.

Using a mechanical test frame, a Laboratory researcher conducts compression tests on plutonium. The diverse material property data collected by materials researchers contribute to the Laboratory's nuclear deterrence mission.

Scientists inspect vials of semiconductor nanocrystals that will be used as single-photon sources and as building blocks for high-efficiency light sources in support of the Laboratory's energy security mission.



A Lab scientist examines the luminescence of a doped scintillator glass under ultraviolet excitation. The work will enable a new class of ultra-compact, low-power radiation detectors and thereby advance the Lab's global security mission.

an otherwise benign environment into an extreme one; and 2) conducting experiments that allow us to explore the full temporal regime may not be possible on a realistic timescale—therefore computation and modeling become critical elements for performance prediction.

In summary, as depicted in the diagram on page 3, our materials strategy is driven by Los Alamos National Laboratory's mission needs for materials with controlled functionality and predictable performance. To design such materials that function even in extreme environments, we manipulate defects and interfaces to our advantage and introduce emergent phenomena to enrich materials' range of behaviors. To succeed in this endeavor, we must excel in a number of areas of leadership. Excellence may span the gamut from profound competency to world leadership, and we enrich our own expertise through strategic partnerships.

Our Areas of Leadership

Complex Functional Materials focuses on materials made of multiple components or building blocks that are physically or chemically bound together to achieve a desired function or response in the resulting system. Thus, complexity manifests itself on the mesoscale and microscale.

Material Resilience in Harsh Service Conditions addresses the evolution of material properties in environments that include static and dynamic stress, radiation, and mechanical, chemical, or thermal extremes. A particular focus is on situations when environments coexist.

Manufacturing Science aims to understand the critical steps in the manufacturing process for the purposes of control and optimization of material properties. The focus lies on understanding the correlations between process, structure, properties, and performance to achieve controlled functionality in the manufactured part.

Actinides and Correlated Electron Materials focuses on understanding and controlling emergent electronic states and predictive performance

Los Alamos Materials Leadership

Exploring the physics, chemistry, and metallurgy of materials has been a primary focus of Los Alamos National Laboratory since its inception. Our Laboratory's proud history of advancing the science of materials includes discoveries instrumental in ending World War II. Subsequent advances in understanding nuclear materials, developing insensitive high explosives, and creating materials for fusion reactions, radiation casings, and neutron sources have enabled a safe nuclear weapons deterrent. The Laboratory's overall materials capability encompasses a budget of $260 million and includes a diverse workforce of approximately 600 personnel. Our materials science expertise has been essential in keeping the world safe for more than 70 years—and it will be vital for a future world with evolving and emerging threats.

of actinide materials. These materials are quintessentially linked by the fact that the physics of actinides—and plutonium in particular—are governed by strong electronic correlations.

Integrated Nanomaterials focuses on two areas. Integration for strategic functionality provides a route to access and control intrinsic nanomaterials functionality for targeted applications and program needs. Integration for emergent functionality provides a route to model, design, and generate multi-material interactions toward creation of emergent behaviors and function not present in the constituent nanomaterials.

Energetic Materials includes explosives, pyrotechnics, and propellants. The focus is on developing means to predict performance and safety characteristics with high fidelity, which requires a detailed understanding of microstructure, dynamics, thermal, and mechanical failure behavior, and the associated high-rate chemistry and shock physics.

Materials Dynamics focuses on understanding structure-properties-performance relationships for the extreme conditions of dynamic loading—encompassing controlled synthesis of materials to meet dynamic performance requirements and requiring computational coupling across length and time scales for three-dimensional microstructure modeling.

Delivering Materials for the Future

Using exascale computing, we envision predicting the ideal defect and interface structure in a material required to yield a set of properties as well as the controlled material synthesis and manufacturing techniques to create those specified structures in the finished product—enabling our materials-by-design vision. Developing the next generation of diagnostics for subcritical experiments requires ECSE, which is enabled by our advances in dynamic materials and energetic materials coupled with next-generation diagnostics and sensors.

To be successful in our vision we have developed MaRIE, our bold conception of a key experimental facility that will address several aspects of materials behavior under extreme conditions. In particular, the proposed capabilities will help characterize the behavior of interfaces, defects, and microstructure at the mesoscale. Advancing the state of the nation's manufacturing capability requires success in our plutonium and uranium strategy, which is enabled by our actinide and manufacturing science.

The execution of the Laboratory's materials strategy will be detailed in the annual implementation plan. That document will lead to success in realizing our 2030 vision (see page 2) for meeting future mission needs.

Both the materials strategy and its implementation plan are living documents. Each area of leadership has a quantifiable end-state goal on a 10-year horizon. As science and technology advance and mission needs shift in the context of the fluid geopolitical climate, we expect this 10-year end state to display agility in order to remain essential to Los Alamos National Laboratory's mission.

Who Should Read This Document

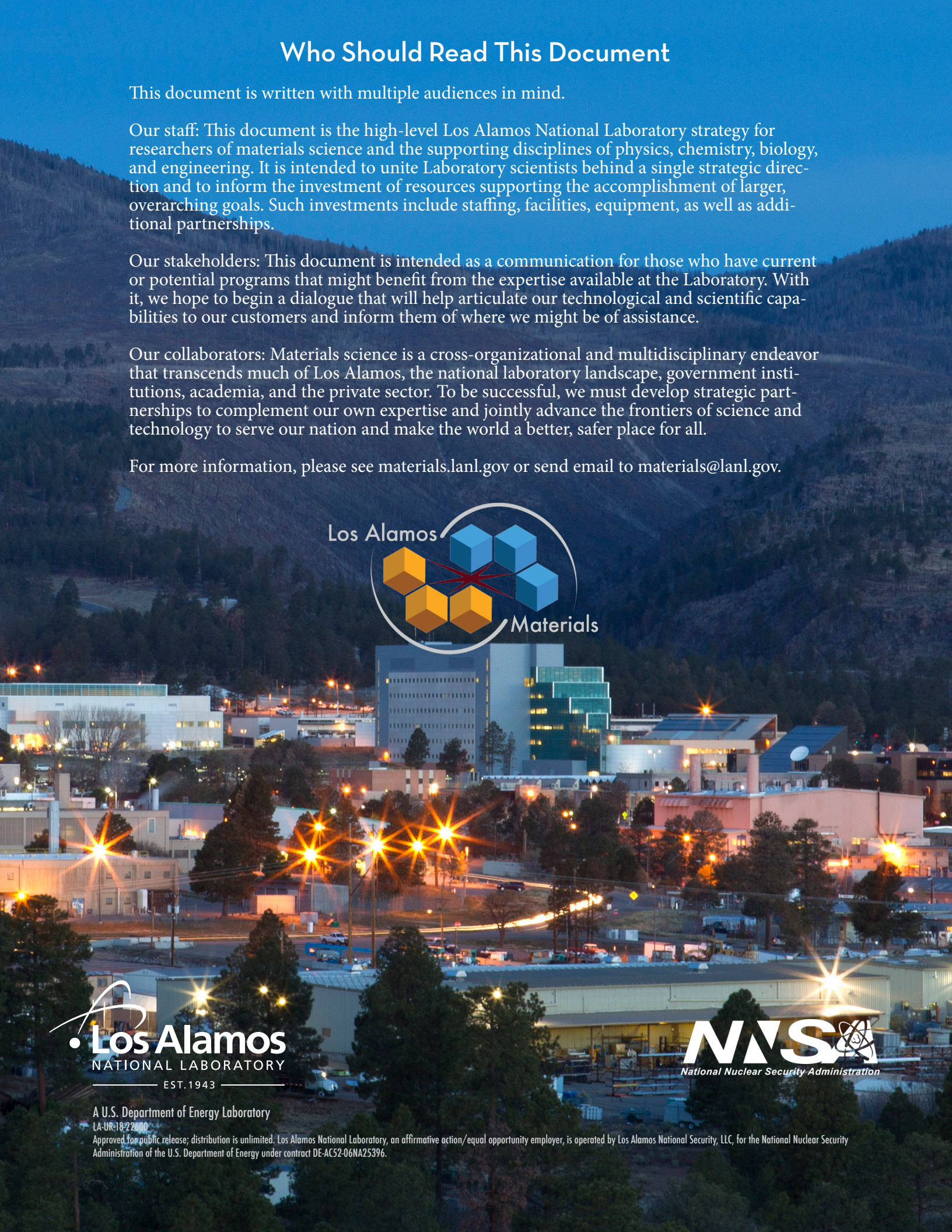
This document is written with multiple audiences in mind.

Our staff: This document is the high-level Los Alamos National Laboratory strategy for researchers of materials science and the supporting disciplines of physics, chemistry, biology, and engineering. It is intended to unite Laboratory scientists behind a single strategic direction and to inform the investment of resources supporting the accomplishment of larger, overarching goals. Such investments include staffing, facilities, equipment, as well as additional partnerships.

Our stakeholders: This document is intended as a communication for those who have current or potential programs that might benefit from the expertise available at the Laboratory. With it, we hope to begin a dialogue that will help articulate our technological and scientific capabilities to our customers and inform them of where we might be of assistance.

Our collaborators: Materials science is a cross-organizational and multidisciplinary endeavor that transcends much of Los Alamos, the national laboratory landscape, government institutions, academia, and the private sector. To be successful, we must develop strategic partnerships to complement our own expertise and jointly advance the frontiers of science and technology to serve our nation and make the world a better, safer place for all.

For more information, please see materials.lanl.gov or send email to materials@lanl.gov.



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