COMPLEX FUNCTIONAL MATERIALS

Complex functional materials are materials comprised of multiple components or building blocks that are integrated or chemically bound together to achieve a desired function or response. Soft materials, such as polymers, as well as structural properties at the mesoscale and micro-scale that control materials function are particularly emphasized in this area of leadership. Further, complex functional materials must generally be developed to satisfy multiple criteria essential to the overall application.

Thus, this area of leadership supports applications that are aligned with all three Los Alamos National Laboratory mission areas of energy security, global security, and nuclear deterrence.

- **Functional materials for a responsive stockpile** include 1) structural components with desired functionalities (mechanical and dynamic properties, aging, rheological behavior) to support the design and stewardship of current and modernized stockpile systems; and 2) in situ and ex situ sensors of radiation, chemistry, load, aging, and other applications for "aware materials."
- **Functional materials for energy conversion and energy storage applications** comprise materials-by-design principles applied for efficient energy utilization, including fuel cells, flow batteries, photovoltaics, solid-state lighting, and carbon capture.
- **Functional materials for chemical, biological, radiological, nuclear, and explosives sensors and detection** focus on chemical and biosensors; tagging, tracking, locating (TTL); and materials that enhance and simplify decontamination.

Los Alamos Leadership in Complex Functional Materials

The multi-component or building-block nature of complex functional materials as defined here encompasses a wide range of materials systems and applications that are not unique to Los Alamos National Laboratory. The Lab's role in this area of leadership ranges from being a leader (materials for a responsive stockpile, fuel cells) to being a fast follower

The Complex Functional Materials area of leadership supports applications that are aligned with all three Los Alamos National Laboratory mission areas of energy security, global security, and nuclear deterrence. Here, a technologist uses a load frame to test the stress/strain properties of a silicone foam.

Materials for the Future

The Los Alamos National Laboratory Materials for the Future strategy derives from our vision to support the Laboratory's national security mission drivers.

We pursue the discovery science and engineering for advanced and new materials to intentionally control functionality and predict performance relevant to ensuring the success of the Lab's missions.

To deliver on our missions, our materials strategy builds on materials science and engineering, enabling the necessary Laboratory leadership in seven key areas:

- Complex Functional Materials
- Material Resilience in Harsh Service Conditions
- Manufacturing Science
- Actinides and Correlated Electron Materials
- Integrated Nanomaterials
- Energetic Materials
- Materials Dynamics

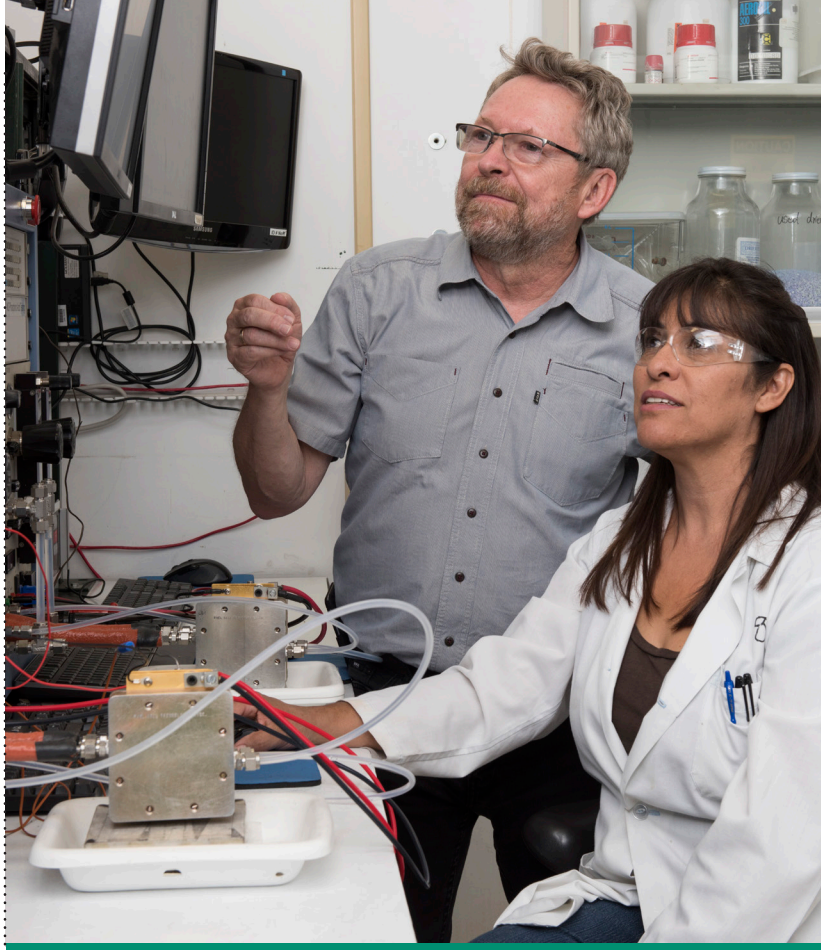
(TTL) or a competent practitioner (flow batteries). For example, Los Alamos has leadership in two multi-lab consortia—the Fuel Cell Consortium for Performance and Durability (FC-PAD) with the Laboratory as lead and the Energy Materials Network Electrocatalysis Consortium (ElectroCat) with Los Alamos as co-lead with Argonne National Laboratory. While the specific applications listed above are Los Alamos mission relevant, discovery science based on the advancement of synthetic methods, characterization, and theory, modeling, and simulation techniques is critical to the continuing success in this area. The development of such techniques can often lead to uncovering the hidden critical characteristics required to understand materials behavior and ultimately control function.

Key Science Questions

- What are the design principles that enable:
  - Manipulation of chemical bonds and structures for tunable chemical interactions and reactions?
  - Control of nano- and meso-structure, morphology, phase, composition, and interfaces?
  - Control of functionality across dimensions?
- How can we control the flow of energy through materials or between material interfaces?
- How do we design, synthesize, model, and simulate adaptive materials across multiple length and time scales?
- How can we design materials with large functional or structural response to small signals?
- Can we exploit defects to create and enhance materials functionality?

10-year End State

Los Alamos National Laboratory efforts in Complex Functional Materials will lead the nation's nuclear weapons complex forward in new predictive materials design. We should be the leader in synthesizing, characterizing, and modeling of soft materials for the nuclear weapons stockpile and be recognized leaders in soft materials by the Department of Energy (DOE) National Nuclear Security Administration (NNSA), as well as the DOE's Office of Science and Office of Energy Efficiency and Renewable Energy. In addition, we will lead the complex in our ability to predict and control materials structure at the mesoscale, where structure at this length scale controls or strongly influences materials properties. We perform a crucial role in the stewardship of soft materials to support the research and design of modern stockpile systems for DOE NNSA. Further, our participation in the DOE's Office of Science and Office of Energy Efficiency and Renewable Energy programs in soft materials is important because it provides essential insights in fundamental science and in applications that go beyond those of the stockpile, while building and maintaining capability that can be utilized by the weapons programs.



Discovery science based on the advancement of synthetic methods, characterization, and theory, modeling, and simulation techniques is critical to the continuing success in this area of leadership. Shown here are staff in a Los Alamos fuel cells laboratory.

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

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