



Theme 2: Renewable energy research, development and deployment Science Program Office – Applied Energy

**Applied Energy overview, including focus on fuel cell program and
history of successful collaboration**

Rod Borup
LANL Fuel Cell Program Manager

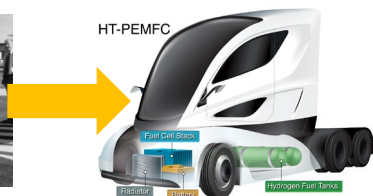
December 3, 2021

Core mission capabilities have contributed to DOE energy missions for decades

Pathways to deployment for transportation

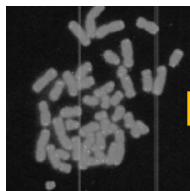


Nuclear rocket program



Electric heavy-duty vehicles

Harnessing algae for bioenergy

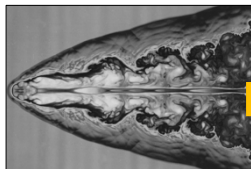


Human Genome Program



Boosting algae productivity

New tools to model complex energy systems

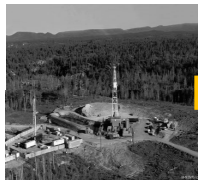


Weapons modeling & simulation

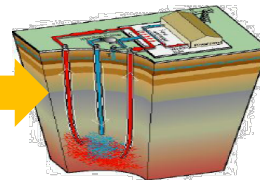


Sub-surface modeling & simulation

Technologies to address GHG emissions



Containment expertise



Enhanced geothermal systems

DOE Applied Energy Programs

Advanced Research Projects
Agency-Energy (ARPA-E)

Cybersecurity, Energy Security,
and Emergency Response (CESER)

Energy Efficiency
and Renewable Energy (EERE)

- Bioenergy Technologies
- Hydrogen & Fuel Cell Technologies
- Vehicle Technologies
- Geothermal Technologies
- Solar Energy Technologies
- Wind Energy Technologies
- Advanced Manufacturing

Office of Fossil Energy (FE)

- Carbon Storage
- Carbon Capture
- Unconventional Gas
- Critical Materials
- Materials in Extreme Conditions

Office of Electricity (OE)

- Advanced Grid R&D
- Energy Storage
- Microgrid R&D
- Grid Modernization

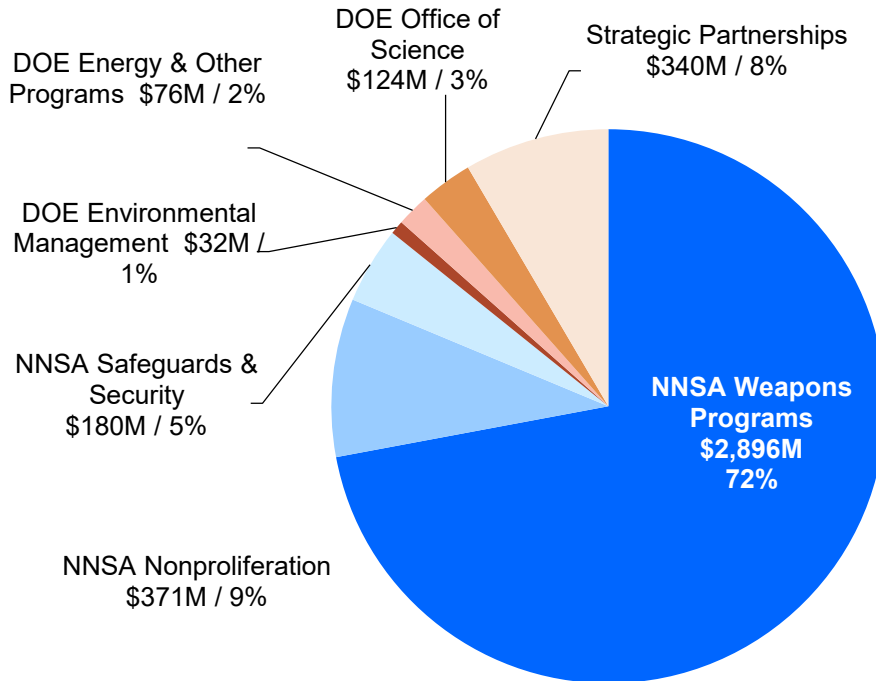
Capability Pillars define six key areas of science, technology, and engineering in which Los Alamos must innovate and excel.

Energy security challenges are prioritized in R&D investments across most Capability Pillars.

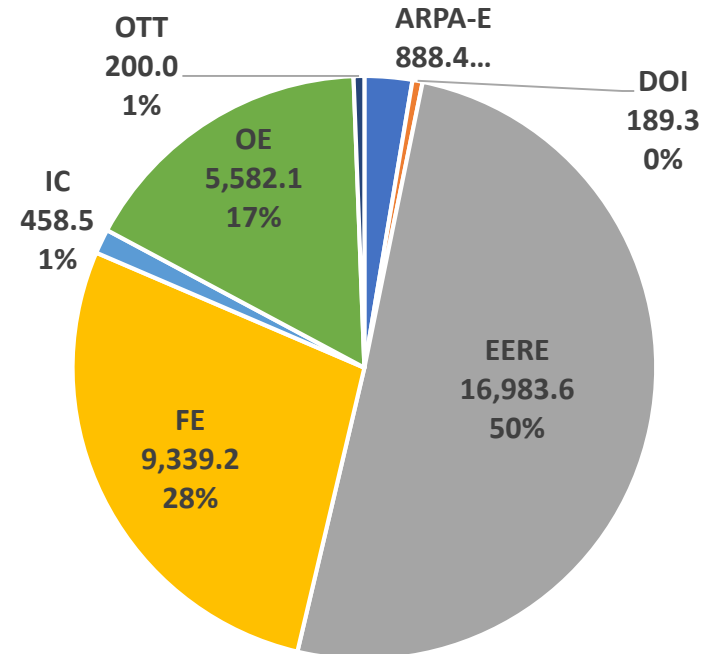
MATERIALS FOR THE FUTURE	Fuel Cells <ul style="list-style-type: none">• Polymer Electrolyte Membrane (PEM) technology• Materials and process development Critical Materials <ul style="list-style-type: none">• Selective extraction of REEs from low-temp geothermal fluids• Co-mingling desalination with the production of critical materials• Hybrid methods for supercritical desalination
NUCLEAR AND PARTICLE FUTURES	
INTEGRATING INFORMATION, SCIENCE, AND TECHNOLOGY FOR PREDICTION	<ul style="list-style-type: none">• Advanced grid modeling• Cyber security for energy delivery systems• Infrastructure Security and Energy Restoration
SCIENCE OF SIGNATURES	Signals from Noise <ul style="list-style-type: none">• Machine learning to extract more knowledge from geophysical signals from geothermal systems and other subsurface environments
COMPLEX NATURAL AND ENGINEERED SYSTEMS	<ul style="list-style-type: none">• Advanced Algae Systems• Feedstock and Logistics• Biomass Conversion• Advanced Development and Optimization
WEAPONS SYSTEMS	

Applied Energy Funding

FY22 LANL
Programmatic Portfolio (est.) = \$4,019M*



SPO-AE Funding (\$K)
FY21 BA - \$33,641.2*
Carryover - \$52,083.7K*



*Many programs forward funded; BA is initial projection

Multi-institutional collaborations are critical to technology development and deployment

National Risk Assessment Partnership (NRAP)



Carbon Capture Simulation for Industry Impact (CCSI²)



Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment (BOTTLE)



Feedstock Conversion Interface Consortium (fcic)



Million Mile Fuel Cell Truck (M2FCT)



Grid Modernization Laboratory Consortium (GMLC)



Los Alamos “Smart Microbial Cell Technology” helps to improve processes to upcycle plastics



Taraka Dale
Consortium Leadership

- High throughput screening expertise
- Strategic planning
- Structuring objectives, tasks, milestones
- R&D prioritization



Ramesh Jha
Technical Leadership

- Computational protein engineering
- Biosensor design and development
- High-throughput screening to enable plastic waste deconstruction and to improve its bioconversion into higher-value product

2020 R&D 100 ENTRY ■
RAMESH JHA, TARAKA DALE, CHARLIE STRAUSS

SMART MICROBIAL CELL TECHNOLOGY

Rapidly Screens and Optimizes Enzymes and Whole-cell Biocatalysts

- ◆ Provides ultra-high-throughput screening
- ◆ Enables fast, direct, and accurate measurements
- ◆ Applies to enzymes, pathways, and microbial strains
- ◆ Reduces labor, material costs, and time requirements

Los Alamos NATIONAL LABORATORY EST. 1943

The poster features a central image of a petri dish containing a dense culture of green fluorescent microbes, held by a person wearing blue gloves. The background shows a person's face in profile, looking at the dish.

Real-time situational awareness and analysis capabilities for energy resilience and national security

North American Energy Resilience Modeling (NAERM)



Russell Bent
Area lead for NAERM natural gas. Area lead for validation, verification, and uncertainty quantification of NAERM models.

NAERM leverages Los Alamos capabilities in infrastructure science to address gas modeling needs

- GasModels.jl developed at LANL
 - Enables computational evaluation of emerging gas network formulations and algorithms in a common platform
- Office of Electricity funded project
 - Efficient infrastructure utilization—improve deliverability of natural gas
 - Gas market design and analysis—value-driven delivery of natural gas

This work informs Defense Critical Electric Infrastructure (DCEI) efforts.

NAERM Software Framework
Delivered September 2019

Natural Gas Hydraulic Modeling Capability
Regional capabilities delivered September 2020

Natural Gas Hydraulic Modeling Capability
Strategy Plan to be delivered Fall 2021

Intermountain West Energy Sustainability & Transitions (I-WEST)

On the road to carbon neutrality in the Intermountain West

Developing a regional **technology roadmap** to transition the Intermountain West to a carbon neutral and economically sustainable energy system, and building a **regional coalition to implement and deploy** the roadmap within the next 15 years.



Place-based Approach

Emphasizes the importance of developing an energy-transition roadmap based on regionally relevant options.



Carbon Neutral Technologies

Focus on technologies that can achieve regional carbon neutrality on an accelerated timeline.



Regional Outreach

Local events solicit input on community's needs, goals, expectations, and concerns pertaining to energy transition.

Hydrogen and Fuel Cell R&D at Los Alamos

- Longest running non-weapons program at LANL (since 1977)

– **The first fuel cells for transportation program**

- The **current DOE HFTO program grew out** of the original Los Alamos program

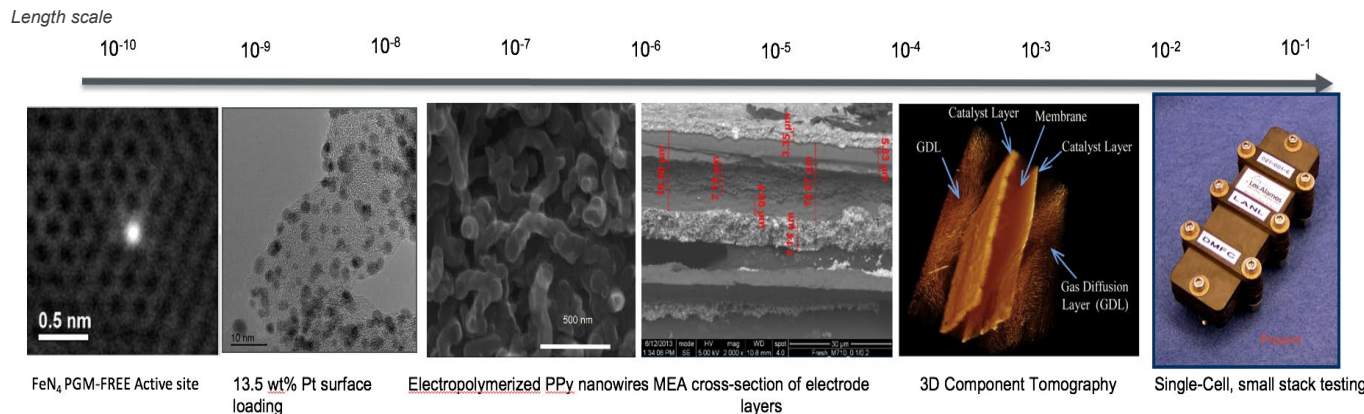
- **LANL Leads Projects That Focus on Stack Components**

- *M2FCT (Million Mile Fuel Cell Truck)*
- *ElectroCat 2.0 Consortia (PGM-free electrocatalysis)*
- *Alternative membranes (Alkaline, High Temperature)*
- *Low-PGM Electrocatalysis*
- *Electrode and MEA Design (Membrane Electrode Assembly)*
- *Water transport (Novel GDL Materials)*
- *Hydrogen Safety Codes & standards; sensors; fuel quality*
- *Miniature Fuel Cell Stacks (NNSA funded)*

Funding

- **DOE EERE HFTO**

- NNSA
- ARPA-E
- CRADAs
- LDRD
- OE
- BES



Strong national lab, university, and industry partnerships key to success in Fuel Cell consortia projects



Rodney Borup (co-lead with LBNL)
Million Mile Fuel Cell Truck (M2FCT)

- Enhancing the performance and durability of polymer electrolyte membrane fuel cells while simultaneously reducing their cost
- Demonstrate world-class improvements in fuel cell performance and durability that exceed the targets set by the U.S. DOE

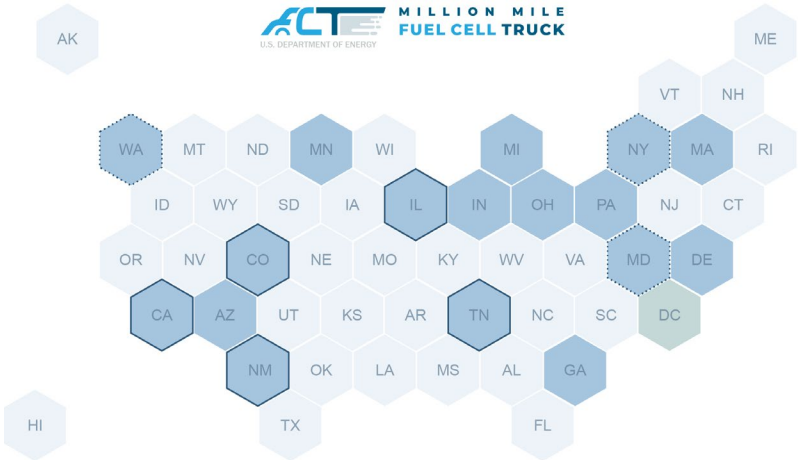


Piotr Zelenay (co-lead with ANL)
ElectroCat 2.0: Energy Materials Network Consortium

- Accelerating development and deployment of platinum group metal-free electrocatalysts in fuel cells and electrolyzers
- Systematic approach combining experiment, theory, machine learning (ML), high-throughput and combinatorial techniques, advanced materials characterization



M2FCT Partners



HD MEA Projects

HD Membrane Projects

HD Stack Projects

Primary Labs	Partners Labs	Partners Academia	Partners Industry
LBNL LANL ANL NREL ORNL	PNNL BNL NIST	Cornell Carnegie Mellon Univ. Colorado School of Mines GeorgiaTech Northeastern University of Tennessee	3M Company Akron Polymer Products Ballard Chemours Cummins General Motors Kodak Lubrizol Nikola Motors Pajarito Powder Plug Power

Discretionary Funding: Recently Announced

- **State University of New York Buffalo**, \$200,000: *Integrating Highly Durable Carbon Supports and Intermetallic PtCo Catalysts for Heavy-Duty MEAs*
- **UC Irvine**, \$175,000: *Materials and Design Solutions for PEMFC Durability*
- **Drexel University**, \$200,000: *Advanced PILBCP Ionomer Composites for Durable Heavy Duty PEMFCs*
- **UC Merced**, \$150,000: *Characterization and Simulation of Interfacial Transport Phenomena in the Membrane-Electrode Assemblies using Rheo-Impedance and Imaging Diagnostic Tools*
- **Florida International University**, \$200,000: *Real-Time Continuous Monitoring of Ionomer Degradation with Ion-Sensitive Field-Effect Transistor (ISFET) Microsensors*

Main Laboratories

Affiliate Laboratories

Inclusion, Diversity, Equity, Accountability

- Diverse group of researchers within the consortium
- Work with disadvantaged communities including HBCUs, HSIs, community colleges
 - ↪ Have various internships for students and targeted discretionary funding
 - ↪ Existing collaboration with NNSA to enhance STEM background & education
 - Including set-up of electrochemistry systems at HBCU's
 - Training, access to cutting-edge research, use of state-of-the-art facilities



Hands-on research



Short Courses/Trainings



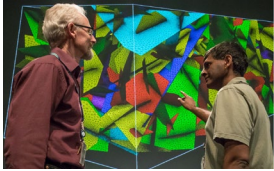
On-site support

- Disadvantaged neighborhoods will be favorably impacted with improvements to long-haul trucking corridors and heavy-duty centers (*e.g.*, ports) *
 - ↪ Greening of the transportation will greatly improve their local emissions and air and noise pollution

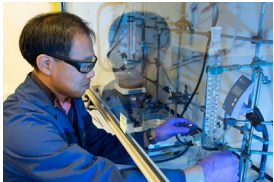
Applied Energy Collaborations with UCI

- M2FCT
 - Catalyst task: Vojaslav Staminchovich
 - Discretionary Call: Plamen Atanassov
- Students
 - Kaustubh Khedekar (Iryna Zenyuk / Spendelow/Borup/Komini-Babu)
 - Andrew Chio (Nalini Venkatasubramanian / Russel Bent) “Integrating Model and Data-Driven Methods in IoT-enabled Resilient Infrastructure”
- UC / Lab Calls
- Other collaborations
 - Plamen Atanassov ~ 19 years on-going
 - Vojaslav Staminchovich
 - Iryna Zenyuk
 - Jack Brouwer

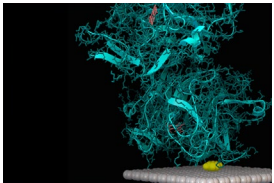
Los Alamos focuses on some key areas of excellence that extend to energy security



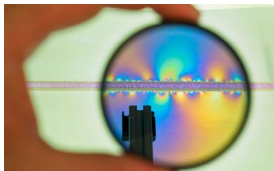
- **Fast, accurate simulation of complex physics (virtual learning)**
(fuel cells; energy storage; advanced materials for power plant)



- **Materials discovery and performance in extreme conditions**
(fuel cells; energy storage; fuel conversion; plastic innovations)



- **Genomics and advanced analytical microbiology**
(advanced algae systems and bioproducts)



- **Engineered subsurface systems**
(shale gas; CO₂ enhanced oil recovery; CO₂ geothermal; CO₂ storage)

Transforming our understanding of the subsurface through real-time visualization, forecasting, and virtual learning



George Guthrie



Rajesh Pawar



Hari Viswanathan



Targets improving real-time decisions for subsurface

- Combines accuracy and predictability of physics with speed of machine learning

New challenges in fossil energy parallel challenges in national-security missions

- New signature identification (small signals, noisy background)
- Rapid prediction for complex, uncertain systems

10-year initiative, launched in summer 2019

- Proof-of-concept phase: 2 years, ~\$20M from both FE-20 & FE-30
- Oil/gas: improve decisions on recovery and economics for fractured reservoirs (e.g., shales)
- Carbon: Improve decisions on monitoring and operations of CO₂ storage

Using data science to reduce time and cost for material development and lifetime predictions

eXtremeMAT



Laurent Capoloungo
Deputy Technical Director &
Modeling and Simulation Lead



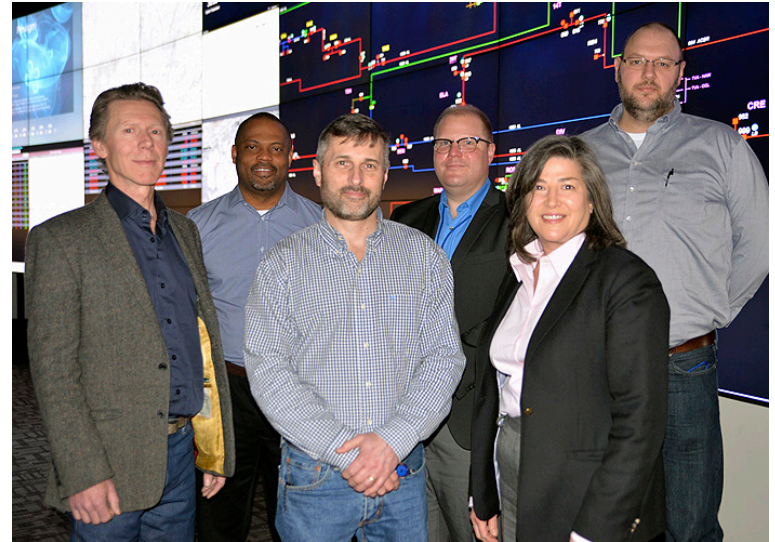
Ellen Cerreta
Steering Committee Member

- Leveraging national lab capabilities in materials design, high-performance computing, manufacturing, and characterization
- Developing and validating computational tools to predict material lifetime performance, which will enable:
 - rapid certification of new materials for use in extreme environments
 - development of new materials with extended lifetimes by understanding the causes behind common material failures
- Engaging with industry to ensure products/models will meet their needs



Research team demonstrates secure communication technology for the nation's electricity suppliers

- Los Alamos and Oak Ridge national laboratories partner with EPB, a community-based utility and telecommunications company serving Chattanooga, Tennessee, to test quantum key distribution (QKD)
- QKD is a quantum-based technology that could improve the cybersecurity, longevity and efficiency of the nation's power grid
- The team has drastically increased the range that these resources can cover in collaboration with their new industry partner, Qubitekk



*Potential new LANL/ORNL collaboration:
Proposal to DOE Office of Science, five-year project, approximately \$12M*