SANDIA REPORT
SAND2020-9986
Printed September 2020

Sandia National Laboratories

A Review of Sandia Energy Storage Research, Capabilities, and Opportunities – 2020 to 2030

Clifford K. Ho, Stanley Atcitty, Stephen J. Bauer, Daniel R. Borneo, Raymond H. Byrne, Babu Chalamala, Joshua Lamb, Timothy N. Lambert, Benjamin L. Schenkman, Erik D. Spoerke, and Jonathan A. Zimmerman

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico
87185 and Livermore,
California 94550

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology & Engineering Solutions of Sandia, LLC.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone:	(865) 576-8401
Facsimile:	(865) 576-5728
E-Mail:	reports@osti.gov
Online ordering:	http://www.osti.gov/scitech

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312

Telephone:	(800) 553-6847
Facsimile:	(703) 605-6900
E-Mail:	orders@ntis.gov
Online order:	https://classic.ntis.gov/help/order-methods/

ABSTRACT

Large-scale integration of energy storage on the electric grid will be essential to enabling greater penetration of intermittent renewable energy sources, modernizing the grid for increased flexibility security, reliability, and resilience, and enabling cleaner forms of transportation. The purpose of this report is to summarize Sandia's research and capabilities in energy storage and to provide a preliminary roadmap for future efforts in this area that can address the ongoing program needs of DOE and the nation. Mission and vision statements are first presented followed by an overview of the organizational structure at Sandia that provides support and activities in energy storage. Then, a summary of Sandia's energy storage capabilities is presented by technology, including battery storage and materials, power conversion and electronics, subsurface-based energy storage, thermal/thermochemical energy storage, hydrogen storage, data analytics/systems optimization/controls, safety of energy storage systems, and testing/demonstrations/model validation. A summary of identified gaps and needs is also presented for each technology and capability.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

EXECUTIVE SUMMARY

Large-scale integration of energy storage on the electric grid will be essential to enabling greater penetration of intermittent renewable energy sources, modernizing the grid for increased flexibility security, reliability, and resilience, and enabling cleaner forms of transportation. Energy storage technology is at a stage where further research is needed to ensure that the technology becomes cost-effective and reaches the technical maturity to become viable across all application markets. Energy storage systems are complex integrated systems that require advancements from materials science, prototype development to system validation and integration into the grid infrastructure.

Sandia has a diverse set of R&D capabilities in energy storage technologies that can help the country transition to clean energy. These energy-storage capabilities are spread across Sandia, including battery materials research, manufacturing, and characterization capabilities in **1500**, **1800, 2500**, and **8800**, and energy-storage technologies for transportation and grid applications in **8300** (hydrogen and fuel cell technologies) and **8800** (geologic storage, concentrating solar power/thermal storage, grid storage systems, power electronics, grid analytics, outreach activities). Additional capabilities exist in **1300** and **5200** that support grid modernization activities.

The DOE Research and Technology Investment Committee has designated energy storage as a grand challenge and strategically important area with significance for global leadership. Our goal is help sustain U.S. leadership in energy storage technologies and manufacturing. We will play a critical role in ensuring that a dynamic, high tech industry can flourish in the country and that US companies are well positioned to supply the emerging worldwide demand for energy storage systems. To achieve these objectives, we will closely work with external partners at national laboratories, universities and U.S. companies to solve critical R&D challenge and advance the development of low-cost energy storage technologies.

Key Capabilities

Battery Storage Technologies: Key capabilities in battery storage technologies include materials synthesis (1800, 8800), characterization and diagnostic capabilities (1512 and 1800), battery assembly and cell prototyping (1800, 8800), cell/system testing facilities (1800, 8800).

Power Electronics and Power Conversion Technologies: Sandia has a number of unique power electronics facilities that develop and analyze conversion systems, wide bandgap semiconductor materials and devices, and advanced capacitors (1000, 5000, 8811). In addition, advanced thermal-to-electric power conversion systems are being researched in 8823 and 8841.

Subsurface Storage Technologies: Sandia has expertise in subsurface site characterization, laboratory and in-situ field testing, complex coupled thermal-mechanical-hydrological modeling of geologic formations, and wellbore life-cycle analyses (8860).

Thermal/Thermochemical Energy Storage: Sandia runs the National Solar Thermal Test Facility (8823), which is the nation's only large-scale concentrating solar power tower test facility, including capabilities to study advanced thermal-storage technologies using molten salts and solid particles.

Hydrogen Storage Technologies: Center 8300 has a number of laboratory capabilities to analyze and develop hydrogen storage and fuel cell technologies, including the Hydrogen Effects on Materials Laboratory, Hydrogen Transport and Transport Laboratory, and Hydrogen-Surface Interactions Laboratory.

Data Analytics, Systems Optimization, and Controls: Key capabilities and software include QuEST, EGRET/Prescient, dynamic modeling of energy storage, and algorithms for wide-area control and optimal dispatch of energy storage (8811). Additional data analytics and deep-learning capabilities exists in the Center for Computing Research (1400).

Safety of Energy Storage Systems: Key facilities to test and evaluate energy storage safety include the Battery Abuse Test Laboratory, Burn site test facility, Battery calorimetry testing, destructive testing, and computed tomography scanning (2500).

Testing, Demonstrations, and Model Validation: Sandia has large-scale testing facilities to demonstrate energy storage systems, include the Energy Storage Controls and Analytics Lab and the Energy Storage Test Pad, which have focused on battery storage technologies (8811). The NSTTF can also be used for large-scale testing of thermal storage technologies.

Key Challenges and Needs

Key challenges, needs, and cross-cutting opportunities for Sandia to serve the large-scale energy storage needs of the electrical grid and transportation sectors include the following:

- **Sandia Gaps and Challenges**
    - Coordinated research efforts across battery research teams to increase engagement and support for OE, JCESR, and LDRD programs
    - Equipment, methods, and capabilities to accelerate materials discovery for battery, thermal, and thermochemical storage technologies and power conversion technologies
    - Expertise and use of machine learning to optimize chemistries and formulations for storage materials (battery, thermal, thermochemical, hydrogen storage media and containment materials)
    - Techniques for low-cost, high-yield fabrication and manufacturing of materials, devices, and components for storage and power conversion
    - Development of facilities and engineered systems that demonstrate scale-up of lab-scale devices and materials with expected performance and reliability
    - Multiscale modeling that can be applied to scale-up of microstructure features and processes to engineered systems; developing appropriate constitutive relations for continuum-based models
    - Development of degradation models that can be incorporated into technoeconomic analyses
    - Development and application of software and tools for life-cycle analyses of energy storage technologies and applications
    - Optimal dispatch algorithms for high penetrations of renewables
    - Evaluation of the reliability and safety of large-scale energy-storage systems, especially batteries; current methods focus on single cells
    - Sharing of information and data with industry and lab partners

- **National Gaps and Challenges**
  - Development of large capacity, long-duration (> ~1 – 100 GWh) energy storage technologies
  - Identification of energy-storage use-case requirements, metrics, and valuation so that appropriate, cost-effective technologies can be researched and developed
  - Technoeconomic analyses including total life-cycle costs (e.g., manufacturing to end-of-life costs and disposition) of various energy-storage technologies for comparison to use-case requirements
  - Safety and reliability standards for large-scale energy-storage systems
  - Integrated energy storage for electrical grid and transportation sectors including fast charging stations, smart-grid controls to enable bi-directional storage using electric vehicles, and real-time accounting for billing and compensation (blockchain opportunities)
  - Infrastructure to enable large-scale hydrogen storage and conveyance

Preliminary Timeline and Roadmap

The timeline for proposed activities described in this report is 10 years, divided into near-term (1 – 2 years), mid-term (3 – 5 years), and long-term (6 – 10 years) objectives. Near-term priorities and activities include taking an active and leadership role within DOE's Energy Storage Grand Challenge initiative and hybrid energy systems activities that address the key gaps and challenges listed above. Sandia can utilize cross-cutting skills across 8000, 1000, and 2000 to identify technologies and methods to enable long-duration energy storage. Mid-term activities and priorities include development of engineered systems and pilot-scale hybrid energy systems with storage and power conversion. Projects focused on low-cost assembly and manufacturing are also needed. The long-term objectives include supporting and implementing transformation of the electric grid to cleaner energy technologies with low-cost, long-duration energy storage. These objectives will also complement and support the transformation of low-emission transportation technologies. Sandia's Laboratory Directed Research and Development (LDRD) program should be leveraged to perform critical research activities that complement these objectives.

ACRONYMS AND DEFINITIONS

Abbreviation	Definition
AC-STEM	Aberration-Corrected Scanning Transmission Electron Microscopy
AES	Auger Spectroscopy
AESI	Advanced Energy Storage Initiative
AFM	Atomic Force Microscopy
ALD	Atomic Layer Deposition
AMO	Advanced Manufacturing Office
APEX	Advanced Power Electronic Conversion Systems Laboratory
ARPA-E	Advanced Research Projects Agency – Energy
ASHES	Automated Sample Handling and Exposure System
BOP	Balance of Plant
BTO	Building Technologies Office
CAES	Compressed Air Energy Storage
CVD	Chemical Vapor Deposition
CSP	Concentrating Solar Power
DAYS	Duration Addition to electricity Storage
DER	Distributed Energy Resources
DETL	Distributed Energy Technology Laboratory
DOE	United States Department of Energy
EBSD	Electron Back Scattered Diffraction
EDS	Energy Dispersive X-Ray Spectroscopy
EERE	Energy Efficiency and Renewable Energy
EES	Electrical Energy Storage
EIS	Electrochemical Impedance Spectroscopy
EMS	Energy Management System
EPMA/WDS	MicroProbe Wavelength Dispersive Spectroscopy
ESCAL	Energy Storage Controls and Analytics Lab
ESGC	Energy Storage Grand Challenge
ESS	Energy Storage Systems
ESTP	Energy Storage Test Pad
FCEV	Fuel Cell Electric Vehicles
FCTO	Fuel Cell Technologies Office (now called HFCTO)
FE	Office of Fossil Energy

Abbreviation	Definition
FIB	Focused Ion Beam
FTIR	Fourier Transform Infrared Spectroscopy
HFCTO	Hydrogen and Fuel Cell Technology Office
HPLC	High-Performance Liquid Chromatography
IA	Industry Acceptance
ISO	Independent System Operator
GPC	Gas Permeation Chromatography
GTO	Geothermal Technologies Office
GW	Gigawatt (10^9 Watts)
JCESR	Joint Center for Energy Storage Research
Kw	Kilowatts (10^3 Watts)
LDRD	Laboratory Directed Research and Development
LMP	Locational Marginal Price
MALDI and ESI	Molecular Mass Spectrometry
Micro-CT	X-ray-based Micro Computed Tomography
MESA	Microsystems Engineering, Science and Applications
MPa	Megapascal (10^9 pascals)
MSEM	Multibeam Scanning Electron Microscopy
MW	Megawatt (10^6 Watts)
NMRS	Nuclear Magnetic Resonance Spectroscopy
NSTTF	National Solar Thermal Test Facility
OE	Office of Electricity (DOE)
PCC	Point of Common Connection
PCM	Phase Change Material
PCS	Power Conversion Systems
PEM	Polymer Electrolyte Membrane
P-FIB	Plasma Forcused Ion Beam
PLD	Pulsed Laser Deposition
POI	Point of Interconnection
RFB	Redox Flow Battery
RFI	Request for Information
RFP	Request for Proposals
RTIC	Research and Technology Investment Committee
SEM	Scanning Electron Microscopy

Abbreviation	Definition
SETO	Solar Energy Technologies Office
SMUG	Solution Mining Under Gas
SPR	Strategic Petroleum Reserve
STEM	Scanning Transmission Electron Microscopy
TEM	Transmission Electron Microscopy
TKD	Transmission Kikuchi Diffraction
ToF-SIMS	Time of Flight Secondary Ion Mass Spectroscopy
TRL	Technology Readiness Level
TW	Terawatt (10^{12} Watts)
UET	UniEnergy Technologies
VTO	Vehicle Technologies Office
WPTO	Water Power Technologies Office
XPS	X-Ray Photoelectron Spectroscopy
XRD	X-Ray Diffraction
XRF	X-Ray Fluorescence
XPS	X-Ray Photoelectron Spectroscopy

SANDIA CENTERS REFERENCED IN THIS REPORT

Center	Name	Energy Storage Research
1300	Radiation and Electrical Science	Grid modernization
1400	Center for Computing Research	Data analytics and deep learning for grid controls (future possibility)
1500	Engineering Sciences	Battery materials research, characterization, modeling
1800	Material, Physical, and Chemical Sciences	Battery materials research, characterization
2500	Component Science, Engineering, & Production	Battery materials research, abuse testing, characterization, manufacturing
5200	Microsystems Engineering, Science and Applications (MESA)	Grid modernization
8300	Chemistry, Combustion and Materials Science	Hydrogen and transportation storage
8800	Energy & Earth Systems	Battery materials research, battery system reliability/safety, testing, demonstration, systems analysis/optimization, data analytics, power conversion, thermal/thermochemical storage, subsurface storage

1. INTRODUCTION AND OBJECTIVES

1.1. Motivation for Energy Storage

Energy storage plays a central role in the rapidly coming convergence across key areas including modernization of the electric grid, electrification of transportation, rapid growth of renewables, and initiatives by states and local bodies towards clean energy technologies.

Large-scale integration of energy storage in electric grid infrastructure has the potential to be transformative. Energy storage can benefit in a number of ways that have bearing on how the future grid operates. These include enabling greater penetrations of intermittent renewable energy sources, providing grid operators a flexible asset that can respond to situations that otherwise are not possible, and enabling cleaner transportation through electrification.

Electrification of transportation is just beginning. Electrification of transportation may require additional investments in grid infrastructure at the residential and commercial level. This could include the need to integrate fast charging infrastructure and the need for new market mechanisms for vehicles to participate in grid services. The impact of electrification of transportation on the grid has focused on cars. However, as electrification extends into fleets, heavy-duty vehicles, business supply chains, and movement of freight, the impacts may be greater than initially predicted. There are currently ~280 million registered vehicles in the United States, and around 15 million registered vehicles in the state of California. If 50% of the vehicles in California are converted to electric vehicles (EVs), and if we assume each vehicle is charged overnight to provide 100 miles of range, which requires ~40 kWh of charge, California would require 7.5 million EVs x 40 kWh/EV = 300 GWh of energy to charge the vehicles each night. This is nearly 40% of the total daily electricity consumption (~800 GWh) in the entire state of California in 2018! Therefore, thousands of "large-scale" battery-storage systems will need to be deployed in California to charge EVs under this scenario if distributed, intermittent renewable energy generation is the dominant source of electricity.

Energy storage will play a major role in integrating renewables and help us to get to a cleaner energy future. As states and cities continue to push towards higher renewable targets with many states moving towards 100% clean energy, the need for low cost energy storage including long duration and seasonal storage becomes significantly more important.

Another area where energy storage can help is in improving the resiliency of electricity infrastructure. When the cost of energy storage drops significantly along with increased lifecycle of energy storage technologies, energy storage can be ubiquitous on the grid – in cars and in garages, at businesses, along highways, and in communities and metropolitan areas. When distributed energy storage assets become pervasive, we may get to a situation where we will have sufficient energy storage capacity to become resilient for various disruptions including weather, natural disasters, and intentional threats. Energy storage can also provide cost-leveling services – consumers can purchase electricity when the price is cheap and then rely on the stored electricity during peak demand periods when prices are higher.

Most of the existing capacity for energy storage in the electricity infrastructure is based on pumped hydro storage plants built over the past forty years to support the operation of nuclear power generation. Recently, modular battery energy storage systems are beginning to grow rapidly. Lithium-ion batteries underpin the growth and development of all forms of consumer electronics and mobility devices. High performance rechargeable batteries are also central to the growth of electric vehicles. And now, grid-scale energy storage systems based on the same Li-ion battery technologies are getting widely deployed in grid-energy storage applications.

The need for energy storage is significant and so is the need for a diverse range of energy storage technologies to satisfy the range of energy storage applications. For example, the US has a base load of about 850 GW and a summer peak of over 1.2 TW. With power generation sources increasingly becoming intermittent with a growing share of solar and wind resources, the need for our power resources to handle intermittency is a growing challenge. With many states legislating renewable portfolio standards and some states firmly moving towards carbon-free generation, the need for energy storage will grow rapidly.

Previous studies have suggested that the decreasing costs of batteries and associated technologies may enable battery systems to meet the short-duration needs of the grid (up to several hours) with high penetrations of intermittent renewable energy systems [1, 2]. However, we currently have a serious gap in addressing "long-duration" energy storage (days to months). Without long-duration energy storage, transitioning the electric grid to fossil free generation will be extremely difficult [3]. In addition, long-duration energy storage will be needed to maintain reserve margins and to maintain the reliability and resilience of the electric grid. Long-duration storage will also ensure resilience of the electrical grid in the face of increasing natural disasters and intentional threats.

Figure 1 shows a chart of current energy storage technologies as a function of discharge times and power capacity for short-duration energy storage. Within the range of short-duration energy storage capacities, applications include reserve and response services (1 – 100 kW), transmission and distribution support grid (100 – 10 MW), and bulk power management (100 MW – 1 GW). Electrical, electrochemical, thermal, mechanical, and hydrogen storage technologies are shown. For large capacity, long-duration storage options, pumped hydro storage, hydrogen, compressed air energy storage, and thermal storage using sensible, latent, or thermochemical methods [4, 5] are seen to be most promising. Commercial concentrating solar power (CSP) has demonstrated the ability to provide on the order of 100 MW of power capacity over 10 hours (~1 GWh) for both grid support and bulk power management.

Thermal storage technologies are also being considered for nuclear power plants to increase the flexibility of these traditionally baseload systems [5]. At times of low or negative electricity prices, heat (or electricity) generated by the nuclear reactor would be sent to thermal storage. At times of high electricity prices, the heat from the reactor and thermal storage would be used to produce maximum electricity output. Generation IV reactors deliver higher temperatures to the power cycle relative to water-cooled reactors, which is beneficial for thermal storage because the required inventory of storage media is reduced. In addition, the higher temperatures enable more efficient thermal-to-electric power conversion.

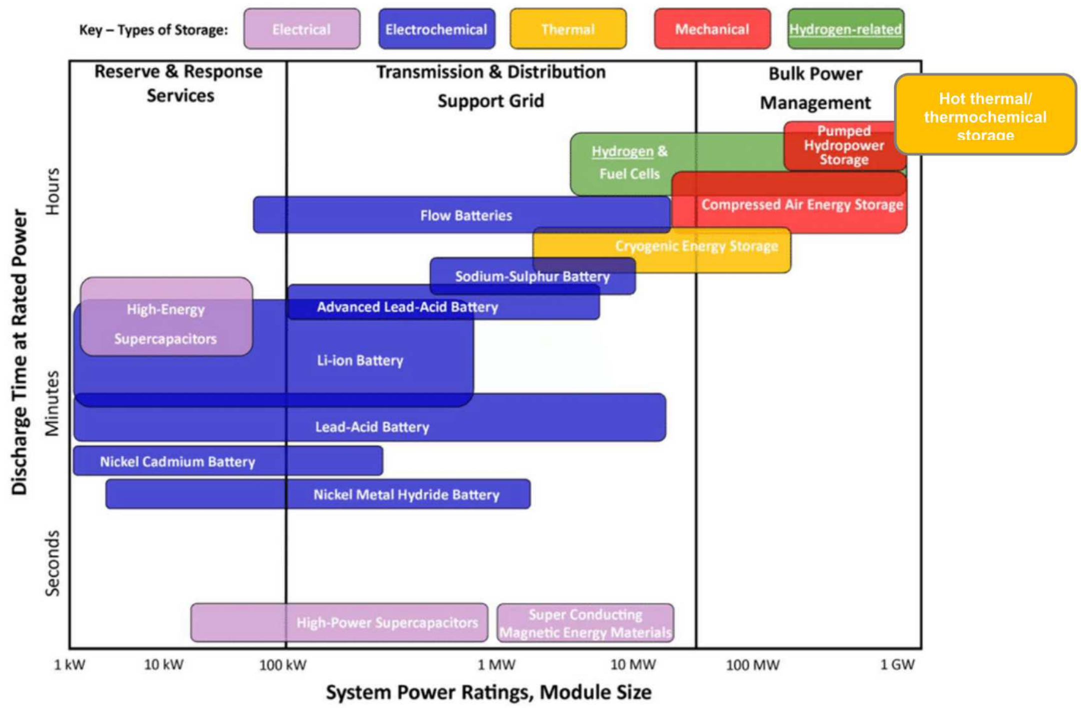


Figure 1. Discharge time and capacity of various energy storage technologies (adapted from [6]; added "Thermal/thermochemical storage."

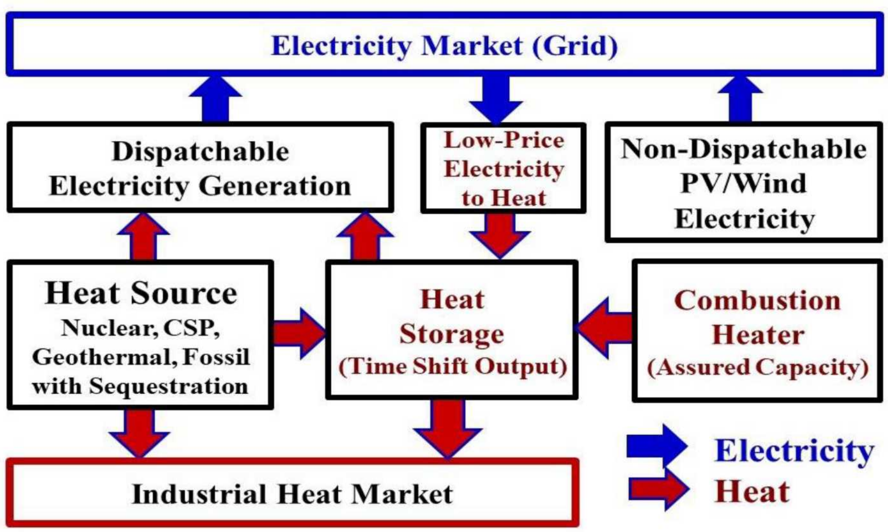


Figure 2. Diagram illustrating how thermal storage can increase the flexibility of traditional baseload power plants [5].

1.2. Energy Storage Research Programs within the U.S.

The US Department of Energy (DOE) has supported a broad range of research programs in energy storage technology. Major programs exist across the DOE program offices. These include EERE Vehicle Technology Office, Water Power Technologies Office, Hydrogen Fuel Cell Technology

Office (HFCTO), and Office of Electricity (OE). Office of Science has supported several Energy Frontier Research Centers (EFRCs) centered on battery energy storage as well the Joint Center for Energy Storage Research. However, the majority of effort was centered around advances in Li-batteries, primarily for transportation applications.

Several recent funding programs in the U.S. have been initiated to address long-duration storage needs. The **U.S. Department of Energy (DOE) ARPA-E** (Advanced Research Projects Agency – Energy) recently awarded 10 projects and nearly $30M for their Duration Addition to electricitY Storage (DAYS) program. The goal is to develop energy storage systems that can provide power to the electrical grid for 10 – 100 hours to increase grid resilience and performance and to enable applications beyond voltage/frequency regulation and intra-day energy shifting. The funded projects will investigate technologies including sensible thermal storage in particles, thermochemical storage, alternative battery and fuel-cell chemistries, thermophotovoltaics, and novel heat pumps and pumped hydro systems. The call sets forth specific levelized cost targets for storage of $0.05/kWh, assuming that the system costs decrease with increasing storage duration. However, this previous call did not address the performance requirements (e.g., power/energy capacity, dispatch profile) for long-duration storage, especially as a function of location, market, and variable percentages of intermittent renewables on the grid.

Similarly, the **DOE Solar Energy Technologies Office (SETO) CSP** program issued a call in their FY19 Funding Opportunity Announcement for proposals on "firm thermal energy storage." The goal is to expand dispatchability and availability of CSP plants to the grid by providing long-term thermal energy storage via sensible, latent, or thermochemical methods. Requirements for the amounts of storage and electricity production were prescribed for weekly and seasonable storage applications, but studies providing information on actual long-duration storage capacity requirements (energy and power) as a function site-specific resources, market, and renewables penetration were not specifically sought.

The **DOE Office of Electricity (OE)** sponsors the **Grid Energy Storage** program, which is focused on the development of advanced energy storage technologies and systems including the development of low-cost battery technologies, safety and reliability of energy storage systems, power electronics and power conversion systems, computational and analytical tools for efficient utilization of energy storage in the electricity infrastructure. On the utility side, the program works with utilities on the deployment and demonstration of new energy-storage systems in grid operations, projects, including the development of methods and tools to evaluate the performance of storage systems, and methods for the optimal utilization of energy storage assets. The program engages staff from several departments across the national laboratories in the materials sciences, power sources, electrical sciences, fire science, power systems, and renewables and grid integration. The program also has significant external collaborations with over 20 US universities, a number of companies in the electricity industry including electric utilities, product developers, and other national laboratories to enable the development and rapid integration of energy storage technologies in the electricity infrastructure. Sandia manages the DOE Energy Storage program archival website, Energy Storage Safety Collaborative, and DOE Global Energy Storage Database for the DOE OE.

Major program areas being funded by the DOE OE Grid Energy Storage program include the following:

- Low cost energy storage technologies including batteries, flywheels
- Power electronics and power converters
- Energy storage safety and reliability

- Energy storage optimization and analytics
- Utility demonstration projects and industry collaboration
- Outreach to state and federal regulators and policy makers

The Advanced Energy Storage Initiative (AESI) is "a coordinated, integrated, and measurable DOE-wide strategy to accelerate the development of energy storage and power system flexibility technologies." The goal is to improve "both bi-directional electrical and thermal energy storage as well as systems supporting electric grid flexibility" for energy generation and consumption. The key elements of energy storage research, development, and deployment include basic science, materials development, applied device and system R&D, development of cost & performance metrics, testing and performance validation, systems analysis and valuation, and market adoption. AESI has links to the Office of Science, ARPA-E, and the Grid Modernization Initiative. Figure 3 shows a summary of the various research areas embodied by AESI.

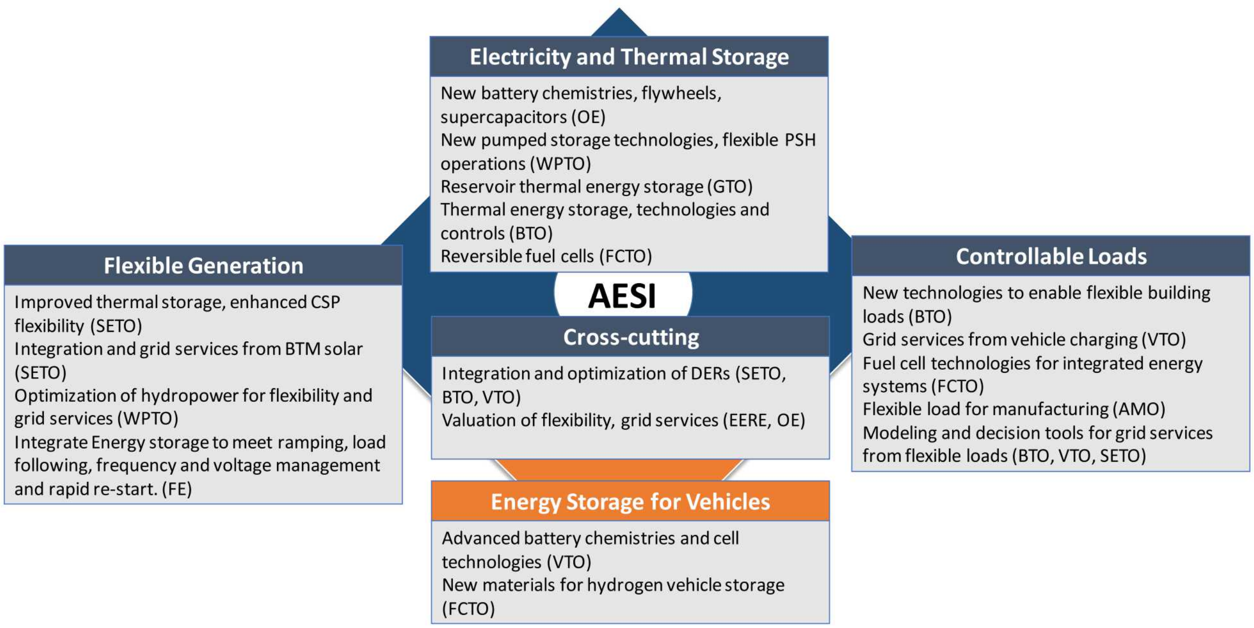


Figure 3. Research areas of DOE's Advanced Energy Storage Initiative (AESI). From presentation by Eric Hsieh (OE) and Alejandro Morena (EERE).

Research and Technology Investment Committee (RTIC) Energy Storage Subcommittee implements the DOE Research and Innovation Act, identifying opportunities "for collaborative research, development, demonstration, and commercial application of innovative science and technologies" through "coordination and consolidation of DOE's existing activities and programs" and "prioritization of activities that use domestic resources." On October 30, 2019, Eric Hsieh presented an overview of the RTIC Energy Storage Subcommittee and its goals. They recommended an **Energy Storage Grand Challenge (ESGC)** with a vision to be the world leader in energy storage utilization and exports by 2030. The mission of the ESGC is to "focus resources from across the DOE to create a comprehensive program to accelerate the development and commercialization of next-generation energy storage technologies and sustain U.S. global leadership in energy storage. The five primary thrusts of the ESGC are as follows (quoted from the 10/30/19 presentation):

1. Technology Development – Establish ambitious, achievable performance goals, and a comprehensive R&D portfolio to achieve them
    a. Area 1 – Near Term Acceleration
        i. Storage Technology
        ii. Balance of Plant
        iii. Market Adoption
        iv. Supply Chain
    b. Area 2 – Long Term Leadership
        i. Storage Science and Technology Advancement
        ii. System-Level Optimization and Innovation (Balance of Plant)
        iii. Supply Chain (overlap with Manufacturing)

2. Technology Transition – Accelerate the technology pipeline from research to system design to private sector adoption through rigorous system evaluation, performance validation, siting tools, and targeted collaborations
    a. Performance validation and demonstration
    b. Financing
    c. Knowledge-sharing and dissemination

3. Policy and Valuation – Develop best-in-class models, data, and analysis to inform the most effective value proposition and use cases for storage technologies

4. Domestic Manufacturing and Supply Chain – Design new technologies to strengthen U.S. manufacturing, recyclability, and reduce dependence on foreign sources of critical minerals

5. Workforce and Technical Assistance – Train the next generation of American workers to meet the needs of the 21stcentury grid and energy storage value chain.

1.3. Objectives

The purpose of this report is to summarize Sandia's capabilities in energy storage and to provide a preliminary roadmap for future efforts in this area that can address the ongoing program needs of DOE and the nation. The roadmap is focused on ways that Division 8000 can integrate and leverage collaborations and capabilities in other areas of Sandia to advance the objectives of DOE's energy storage program. Mission and vision statements are first presented followed by an overview of the organizational structure at Sandia that provides support and activities in energy storage. Then, a summary of Sandia's energy storage capabilities is presented, including hardware and software development, systems analysis, data analytics, controls, testing, and model validation. A summary of identified gaps and needs is presented, followed by a timeline of opportunities based on Sandia's capabilities and current and anticipated needs in energy storage.

2. MISSION AND VISION STATEMENTS

2.1. Mission

Sandia will pursue energy-storage R&D over the next 20 years that includes development of advanced materials for low cost battery technologies, new materials and technologies for long duration and seasonal energy storage, conversion systems to improve the cost and operational performance of power conversion systems, hybrid systems that utilize energy storage to optimize system performance, advanced modeling, software and controls for storage enabled distribution and transmission systems, research on improving safety and reliability, systems analysis, and test demonstrations and model validation to develop solutions for all grid energy storage needs that enable a clean, secure, resilient electric grid.

2.2. Vision and Goal

Sandia will assist DOE in its goal to become a world leader in energy-storage technologies, manufacturing, and supply chain by 2030. Large-scale integration of energy storage in the electric grid will be essential for a cleaner and resilient electric grid. Energy storage technology is at a stage where further research is needed to ensure that the technology becomes cost-effective and reaches the technical maturity to become viable across all application markets. Energy storage systems are complex integrated systems that require advancements from materials science, prototype development to system validation and integration into the grid infrastructure.

2.3. Sandia Energy Storage Research and Centers

Sandia has a diverse set of R&D capabilities in energy storage technologies that can help the country transition to clean energy. These energy-storage capabilities are currently spread across Sandia (see summary of current Centers in Table 1), including battery materials research, manufacturing, and characterization capabilities in **1500**, **1800**, **2500**, and **8800**, and energy-storage technologies for transportation and grid applications in **8300** (hydrogen and fuel cell technologies) and **8800** (geologic storage, concentrating solar power/thermal storage, grid storage systems, power electronics, grid analytics, outreach activities). Additional capabilities exist in **1300** and **5200** that support grid modernization activities.

The DOE RTIC has designated energy storage as a grand challenge and strategically important area with significance for global leadership. Our goal is help sustain US leadership in energy storage technologies and manufacturing. We will play a critical role in ensuring that a dynamic, high tech industry can flourish in the country and that US companies are well positioned to supply the emerging worldwide demand for energy storage systems. To achieve these objectives, we will closely work with external partners at national laboratories, universities and US companies to solve critical R&D challenges and advance the development of low-cost energy storage technologies.

Table 1. Current Sandia Centers supporting energy storage research.

Center	Name	Energy Storage Research
1300	Radiation and Electrical Science	Grid modernization
1400	Center for Computing Research	Data analytics and deep learning for grid controls (future possibility)
1500	Engineering Sciences	Battery materials research, characterization, modeling
1800	Material, Physical, and Chemical Sciences	Battery materials research, characterization
2500	Component Science, Engineering, & Production	Battery materials research, abuse testing, characterization, manufacturing
5200	Microsystems Engineering, Science and Applications (MESA)	Grid modernization
8300	Chemistry, Combustion and Materials Science	Hydrogen and transportation storage
8800	Energy & Earth Systems	Battery materials research and system reliability/safety, testing, demonstration, systems analysis/optimization, data analytics, power conversion, thermal/thermochemical storage, subsurface storage

2.4. Timeline

We are looking at opportunities for a 10-year roadmap with a vision to drive success in several key areas. In the near term (1 – 2 years), we see significant opportunities to leverage initiatives such as DOE's Energy Storage Grand Challenge. In the medium to longer term (3 – 10 years), the coming convergence of grid modernization, vehicle electrification, and activities related to domestic manufacturing will offer additional opportunities to develop new national capabilities for energy storage at scale. Additional details of recommended tasks and priorities for Division 8000 are summarized in Section 4.

- **1 – 2 years**
    - Position Sandia as key player and leader in DOE's Energy Storage Grand Challenge initiative
        - Hold workshops, multi-lab meetings, etc.
        - Implement and expand our capabilities in energy storage technologies and grid analytics/optimization by integrating resources to address the key gaps and challenges listed in Section 4.2
    - Integrate synergistic capabilities in 8000 and other Sandia divisions to enable long-duration storage and hybrid energy systems (e.g., flow batteries, CSP/thermal, chemical, hydrogen, geologic, nuclear, wind, PV)
        - See key gaps and challenges in Section 4.2
- **3 – 5 years**
    - Engineer and demonstrate pilot-scale hybrid energy systems with storage to address key gaps and challenges in Section 4.2
    - Develop large-scale national capabilities in power converters

- Power electronics for batteries, fuel cells, and grid interface
    - Advanced heat engines (e.g., supercritical CO_2 Brayton cycle) for thermal-to-electric conversion
  - Develop capabilities to support low-cost manufacturing of energy storage technologies
    - Materials discovery and process development
    - New processes for effective utilization of materials at large scales
- **5 – 10 years**
  - Support transformation of the electric grid to cleaner energy technologies with low-cost, long-duration energy storage at scale
    - Reliable, safe, low-cost, long-duration energy storage technologies
    - Security and resilience of storage-enabled grids
    - Capabilities to validate integration of new technologies into the future grid
  - Support transformation of low-emission transportation
    - Electrification of transportation and associated storage requirements
    - Hydrogen fuel-cell technologies, production, and storage

3. SANDIA ENERGY STORAGE CAPABILITIES

3.1. Battery Storage and Materials (Erik Spoerke, Org. 1816, and Timothy N. Lambert, Org. 8824)

3.1.1. Battery Storage Technology – Background

Battery storage and materials at Sandia are studied across a wide range of chemistries, systems, and applications, and across scales ranging from molecular design in the laboratory to testing of 1MW battery systems. The breadth of these activities involves significant development of technical capabilities and expertise across multiple centers including 1500, 1800, 2500, 8300, and 8800, making Sandia a unique, multidisciplinary, integrated institution to research battery-based energy storage.

The requirements of the end user strongly influence the nature of the batteries studied or developed and the target performance metrics needed. Batteries may be primary (single use) or secondary (rechargeable) and intended for long term storage, short duration (minutes or less) discharge, or longer-duration discharge (hours). Their applicability includes mobile storage (e.g., vehicles or portable electronics) as well as grid-scale storage, and as a function of their application, they may be exposed to variable chemical or thermal environments. The capabilities at Sandia are designed to enable state-of-the-art syntheses, materials characterization, battery prototype assembly and testing, and performance evaluation, including under abusive conditions. Sandia's mission focus includes a significant effort on battery-based energy storage, including facilities and expertise to explore primary thermal batteries as well as a number of secondary battery technologies. The DOE Office of Electricity funds a significant effort at Sandia, supporting R&D in redox flow batteries (RFBs), zinc-manganese oxide (Zn-MnO_2) alkaline batteries, molten sodium batteries, and more recently, lithium-sulfur batteries. These efforts predominantly emphasize developing basic understanding of the materials chemistry to enable ultimate advancement of these storage technologies for grid-scale energy storage.

Sandia is also a primary contributor to the DOE-funded Joint Center for Energy Storage Research (JCESR), focusing on transformative materials for energy storage. Specifically, JCESR efforts combine experimental and computational efforts to explore several key aspects of new battery systems, aimed at exceeding energy, power, and lifetime limits of conventional lithium-ion and redox flow technologies:

- Electrolytes capable of targeted solubility, ion transport, radical ion stability and electrochemical stability at energy and power density limits
- Electrode interfaces capable of promoting ion desolvation and ion accommodation
- Electrode interphases tuned for enhanced multivalent cation transport and zero parasitic losses plus regenerable carbon surfaces for fast and efficient charge transfer

Finally, there is significant investment from Sandia's LDRD program to solve problems and develop materials for new batteries or to improve critical problems with existing batteries. Recently, Sandia has supported several programs related to metal-air batteries, Zn-MnO_2 and lithium or lithium-ion batteries including:

- Developing Next Generation Electrocatalysts (Energy and Climate LDRD)
- Exploring Reversible Manganese Oxide cathodes for Zn/MnO_2 (Energy and Climate LDRD)

- Exploring high lithium storage capacity carbons and silicon-carbon composites (New Ideas LDRD).
- Investigating the effects of engineered stress on high energy density lithium metal anodes (Materials Science LDRD).
- Investigating new battery materials and fabrication techniques that could enable future national security applications (National Security Programs LDRD).
- Customizable high energy density lithium batteries tuned for Sandia's missions (Grand Challenge).

Additional LDRD programs in past years have also explored novel cathode materials for lithium ion batteries, biomimetic battery systems, numerous modeling efforts to explore solvation, ion transport, and cell design, and even advanced *in situ* studies of lithium ion electrode materials.

Although Sandia conducts significant independent battery research, there is substantial engagement with other national laboratories, industry partners, and academic institutions to expand the scope of technical expertise available to the program. The DOE-OE program examining Zn-MnO_2 batteries provides an excellent example of this collaborative mindset, engaging 4 universities [City University of New York Energy Institute (NY), New Mexico State University (NM), Northeastern University (MA) and Stony Brook University (NY)] and an industrial partner [Urban Electric Power (NY)] to provide a mix of basic research and applied engineering in support of this effort.

Battery materials research requires strong expertise in a number of technical areas including Materials Synthesis, Advanced Characterization, Battery Assembly and Prototyping, and Battery/System Testing.

3.1.2. Battery Storage Technology – Sandia Capabilities

Materials Synthesis

Sandia maintains a comprehensive collection of materials synthesis capabilities that enable study or development of essentially every element of a battery.

Organic and molecular synthesis capabilities enable the study of novel active species, for example in redox flow batteries, or additives to prevent secondary reactions in lithium ion or alkaline Zn-based batteries. Synthesis of bioinspired materials and methods enable novel new, biomimetic energy storage systems. Significantly, there also exists critical expertise in polymer synthesis and processing. These polymeric materials are used as battery seals and separators. Developing novel, selective separators is one of the primary objectives of the Office of Electricity effort on RFBs and Zn-MnO_2. Sandia maintains capabilities to design, synthesize, purify, and cast these materials to form novel separators for controlled ion transport.

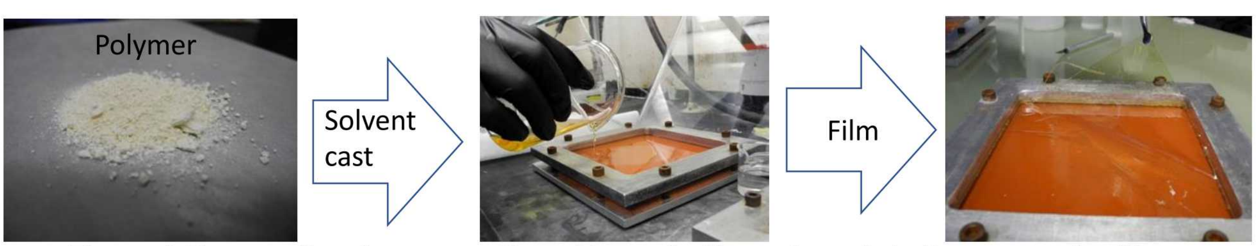


Figure 4. Process flow for preparation of ion-selective polymeric battery separator films.

Solid state battery materials are often formed through solution-phase chemistry using methods such as bulk precipitation, ligand-assisted precipitation, sol-gel chemistry, microwave-assisted synthesis, or solvothermal synthesis. Sandia laboratories maintain necessary expertise and resources to safely synthesize these materials at variable temperatures or pressures, in different solvents, or under controlled atmospheres (e.g., glove box or Schlenk line). These custom materials can then be purified and processed either for solid-state reactions or for incorporation into composite structures.

Solid state chemistry enables the production of lab-scale ceramics and glasses. These materials may be used as solid-state ion conducting separators, seals, or electrode materials. Metallurgical expertise can also be applied for the formation of seals, welds, or current collectors and can be important aspects dictating the final packaging of the batteries. Sandia has decades of expertise and an extensive team of experts capable of synthesizing, processing, and characterizing these solid state materials.

Vapor phase synthesis of thin films or particles is another capability that not only enables novel material development, but also facilitates microelectronic systems integration with batteries or research into micro-batteries and thin film batteries. Chemical Vapor Deposition (CVD), Atomic Layer Deposition (ALD), Pulsed Laser Deposition (PLD), and sputtering are among key tools that can be utilized either as "stand-alone" techniques, or integrated with the Microsystems Engineering, Science and Applications (MESA) fabrication facilities on site at Sandia.

Characterization and Diagnostic Capabilities (1800 and 1512)

Sandia maintains a full suite of characterization capabilities that are central to characterizing new materials during battery development but also used to evaluate materials during "post-mortem" analyses of tested batteries to understand critical relationships between composition, structure, and performance. Relatively smaller capabilities are often distributed within individual laboratories, while larger, more capital intensive equipment (XRD, TEM, SEM, FIB, XPS, etc.) are more centrally maintained, for example in the Materials Characterization department (1819), in the Diagnostic Science and Engineering department (1512) , or even through user proposals within the Center for Integrated Nanotechnologies (CINT, 1880), accessible through user proposals. New equipment and capabilities are regularly added to Sandia's arsenal of characterization tools, but many of them are listed here:

Sample Preparation

- Cleaning Lab
- Metallography Lab
- Focused Ion Beam (FIB)
- Plasma FIB (P-FIB)
- HPLC (analytical and preparatory)

Surface Topography

- Profilometry
- Interferometry
- Atomic Force Microscopy (AFM)

Optoelectronic and Electrochemical Analyses

- Electrochemical impedance spectroscopy (EIS)

- Linear and Cyclic Voltammetry
- Galvanostatic and Potentiostatic characterization
- Dielectric, Ferroelectric,, Piezoelectric, and Magnetic Properties
- Kelvin probe
- UV-Vis Spectroscopy
- Fluorescence
- Photoemission Electron Microscopy
- Differential Electrochemical Mass Spectroscopy

Microstructural Imaging & Analysis

- Comprehensive Optical Microscopy
- Fluorescence and Confocal Microscopy
- Scanning Electron Microscopy (SEM)
- Multibeam SEM (mSEM)
- Electron BackScattered Diffraction (EBSD)
- Transmission Kikuchi Diffraction (TKD)
- Transmission Electron Microscopy (TEM)
- Scanning Transmission Electron Microscopy (STEM)
- Aberration-Corrected STEM (AC-STEM)
- X-ray Diffraction (XRD)
- X-ray-based Micro Computed Tomography (Micro-CT)
- Light scattering and Zeta-potential

Figure 5. Scientists Paul Kotula and Ping Lu working with the aberration-corrected STEM for atomic scale chemical imaging.

Compositional Analysis

- Auger Spectroscopy (AES)
- X-ray Diffraction (XRD)
- X-ray Fluorescence (XRF)
- X-ray Photoelectron Spectroscopy (XPS)
- Energy Dispersive X-Ray Spectroscopy (EDS)
- MicroProbe Wavelength Dispersive Spectroscopy (EPMA/WDS)
- Molecular Mass Spectrometry (MALDI and ESI)
- Gas Permeation and Liquid Chromatography (GPC and HPLC)
- Time of Flight Secondary Ion Mass Spectroscopy (ToF-SIMS)
- Nuclear Magnetic Resonance Spectroscopy
- FTIR and Raman Spectroscopies

Battery Assembly and Cell Prototyping

The requirements and capabilities needed for assembly or prototyping vary significantly by battery chemistry. Fundamental cell-based studies typically rely on assembly in individual laboratories. While this approach does not favor large-scale manufacturing, it does allow for agility in developing and tailoring systems for many different battery assembly strategies.

Relatively conventional cell designs or chemistries can be assembled in small lots or as individual cells, taking advantage of more than 60,000 sq. ft of lab and prototyping space and 10,000 sq. ft of dry room space. These facilities include equipment for powder processing, pressing, mixing, electrode formulation and coating, roll-to-roll coating, welding, winding, component machining, as well as cell assembly and sealing. 3D printing capabilities allow for flexible cell designs, novel prototypes, and agility across a wide range of battery chemistries and cell designs.

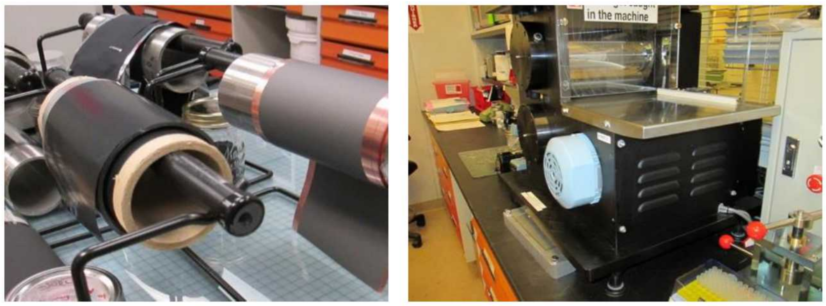


Figure 6. Electrode coating and preparation capabilities for cylindrical battery assembly.

For less conventional or emerging battery chemistries, capabilities exist within individual laboratories to manage sensitive chemistries or unusual cell designs. For example, in support of the DOE OE program, highly air-sensitive metallic sodium-based batteries are assembled individually using custom cell designs in an argon glove box. Alkaline Zn-MnO_2 batteries are also assembled in-house on the benchtop, as they do not require such rigorous atmospheric controls. Electrodes used in this case are typically fabricated on a small scale but are very similar in composition to those produced in higher throughput by industry. A collaboration with Urban Electric Power (NY) provides a path forward to larger-scale assembly for promising results developed in the laboratory. Flow batteries are also readily assembled and characterized at Sandia, where facilities are set up for both aqueous and non-aqueous flow battery chemistries. One special consideration is that although these batteries are studied on a laboratory scale, flow battery test designs have been developed, prototyped, and implemented to allow for true flow-based evaluation of different redox-active molecules, electrolytes, and separators.

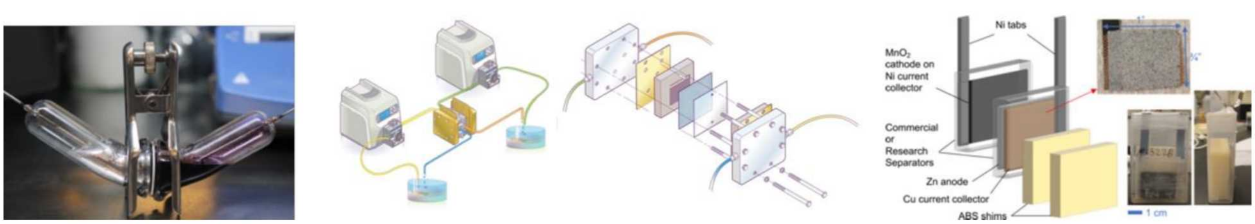


Figure 7. Left: Photograph of a custom molten Na-battery test structure, shown with molten sodium anode and molten salt catholyte. Middle: Schematic of a flow battery test configuration used for aqueous and non-aqueous flow battery testing. Right: Schematic of prototype Zn-MnO_2 cell, picture of a Zn anode and assembled cell used for materials development.

Another valuable set of capabilities relates to Sandia's additive manufacturing capabilities. A variety of direct-write printing platforms and scalable printing tools have enabled materials research to be tightly integrated with functional prototyping. Precision extrusion casting of pastes, slurries, and thermoplastics enable ceramic and polymeric component fabrication while aerosol inkjet, flexographic, and gravure printing techniques are deployed for electronic and electrochemical component research. These capabilities not only include the tools to apply these methods, but also the expertise to develop new molecular and nanoparticle "inks" for printing functional materials, but also to tune processing conditions for unique applications such as low temperature sintering or fine detail prototyping. In addition, state-of-the-art coating printing technologies greatly increase throughput of printed devices with routes that are adaptable to roll-to-roll manufacturing. These new capabilities include slot-die/flexographic coating and micro-gravure printing that can print/coat multiple, registered layers at overlay precision less than 10 microns and print feature sizes down to two microns, thus greatly improving printed electronics efficiencies. These systems are expected to enable new thin and thick film batteries by combining writeable metals, semiconductors, dielectrics, electrolytes, catalysts and enzymes.

Cell/System Testing Facilities:
Individual laboratories across Sandia are involved in testing with a widely varied collection of electrochemical workstations and battery test stations. Laboratories commonly adapt their testing configurations to use multichannel battery testers and incorporate glove boxes to control atmospheric conditions for air-sensitive battery assemblies.

Figure 8. Left: Argon-filled glove box and multichannel battery tester used for laboratory-scale testing of battery performance and reliability. Right: 96-channel battery tester workstation with numerous Zn-MnO_2 batteries undergoing evaluation.

Larger cell systems can be tested, for example through the Power Sources Research and Development department (2546) or the Energy Storage Technology & Systems department (8811). Through these capabilities, it is possible to evaluate battery to module performance, cell reliability, and high precision testing for cycle-life assessment. Large scale systems can be tested on variable scale from 5 kW to 1MW using 480 VAC (3 phase). 1MW/1MVAR load banks are available for either parallel microgrid or series UPS operations, and sub-cycle metering in feeder breakers can be used for system identification and transient analysis. Additionally, thermal imaging can be used to assess system thermal profiles during operation. See Sections 3.7 and 3.8 for more details.

3.1.3. Battery Storage Technology – Gaps, Challenges, and Needs

Although Sandia does maintain a significant collection of resources and works across a number of important technical areas, there remain several areas where Sandia's battery research efforts could be improved and enhanced.

First, research efforts often remain relatively segregated, often based on funding sources. There is opportunity for significant improvement of communication across different battery research "teams." For example, increased engagement between OE programs, JCESR, and LDRD programs and increased interaction, as allowable according to program sensitivity, between mission-based and non-mission research would help eliminate duplication of efforts or equipment, access more Sandia expertise, and research progress in a more cohesive battery research community.

From a capability perspective, much of the battery research is focused on small, laboratory scale systems at a relatively low technology readiness level (TRL). These lab-scale efforts are well-suited to fundamental studies or investigation of existing battery capabilities. Laboratory-supported capabilities to scale laboratory work to demonstration scale (10 kWh-scale) are not yet well-established at Sandia and are typically cost-prohibitive and excessively time-consuming for a single project or principal investigator. Developing these capabilities would require physical space to run these systems, power electronics, and battery integration resources, and manufacturing tools are needed to create and assemble larger quantities of developing battery materials and components. Some of Sandia's aforementioned capabilities in manufacturing and device prototyping could be leveraged to accelerate this effort. It would, however, also require addition of personnel and expertise needed to engineer these systems. Capable as they may be, R&D scientists are not always well-trained to efficiently engineer these larger systems. These personnel could potentially also contribute significantly to mission-related work, where more advanced manufacturing and prototyping may already be more commonplace.

Adding these scaling capabilities would have several important benefits. First, it would add an important new angle to laboratory research efforts, directing the fundamental R&D to consider practical issues of scalability. Second, successful demonstrations of Sandia-developed battery technology would help attract industry collaborators, who are typically reluctant to engage without prototype demonstrations. The lack of industry or commercial engagement continues to limit potential follow-on work to short term research (e.g., LDRD) and restricts the ultimate utilization of non-mission-specific Sandia technologies that are more mature. Finally, the ability to create larger scale systems will be important aspects of a more substantial large-scale, long-duration storage effort at Sandia. Long-duration storage (days to weeks) is an underdeveloped set of technologies where Sandia has the opportunity to establish a leadership position in the coming years. Research capabilities aimed at larger-scale battery development would help advance this initiative.

3.2. Power Electronics (Stan Atcitty, Org. 8811)

3.2.1. Power Electronics Technology – Background

Power conversion systems (PCS), sometimes referred to and used interchangeably as power electronics, are a key enabling technology for energy storage.[1] In a grid-tied energy storage system, the PCS controls the power supplied to and absorbed from the grid, simultaneously optimizing energy storage device performance and maintaining grid stability. There are multiple types of energy

[1] Power electronics as described here are not applicable to thermal storage systems utilized by thermal power stations (e.g., for concentrating solar power technologies) since AC power is produced directly from the power cycle.

storage technologies, and each has their own characteristics and control parameters that must be managed by the PCS. An energy storage installation may be tasked with a variety of different grid support services; the PCS is responsible for controlling the flow of energy to meet the requirements of the intended grid support application.

The major electrical components of a PCS are semiconductor switches, capacitors, magnetic devices such as inductors and transformers, and a controller as shown in Figure 9.

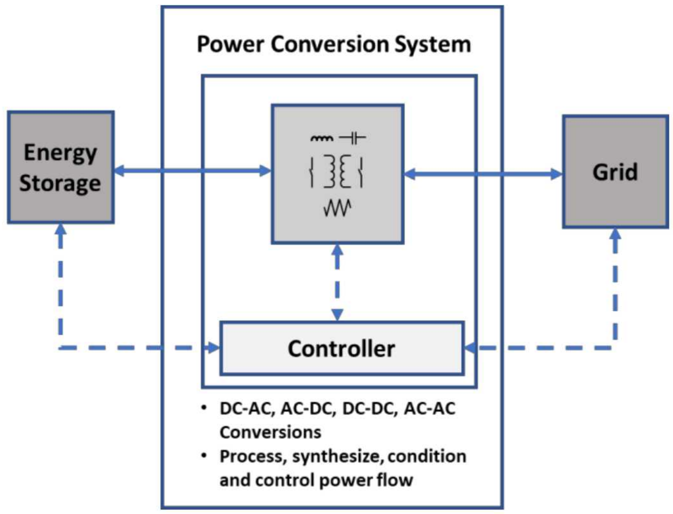


Figure 9. Basic block diagram of a PCS interfacing energy storage with the electric utility grid.

PCS performance continues to increase due to the advancement of material technologies. Traditional PCS for energy storage use silicon-based semiconductor switches. In the past two decades or so, there has been increased interest in the utilization of wide bandgap semiconductor materials such as silicon carbide or gallium nitride. These devices can significantly improve the performance of PCS by increasing power density and power conversion efficiency. Likewise, new materials are enhancing the performance of passive components. Advanced dielectrics and magnetic core materials enable operation at higher temperatures and switching frequencies, increasing both efficiency and reliability. These new materials have the potential to completely transform current power conversion design and control methods.

3.2.2. Power Electronics Technology – Sandia Capabilities

Sandia has an established history of research in power electronics materials, components and systems for multiple applications in weapons, military, transportation, satellites, energy, etc. As a result, multiple laboratories were developed over time to address changing mission requirements. Table 2 highlights key laboratories focused on power electronics and power conversion systems for grid energy storage.

Table 2. Summary of PCS facilities and capabilities for grid storage.

Facility	Description
Advanced Power Electronic Conversion Systems Laboratory (APEX) 	New power conversion system solutions are needed to support the expanding role of energy storage in the grid. This lab supports the development of new power conversion topologies and intelligent controls. Key lab capabilities include real-time simulations, rapid prototyping and electrical fabrication, hardware verification in a unique 30 kW bidirectional testbed. The testbed is a comprehensive test environment for energy storage applications, including storage device emulation at the system, module, and cell level, fault insertion capabilities, and extensive thermal and electrical instrumentation.
Wide Bandgap Semiconductor Material and Device Characterization Laboratory  	Semiconductor devices are considered heart of power conversion system. They determine to power conversion system performance, reliability and cost. Wide Bandgap semiconductors will significantly impact future power conversion design. With any new materials, there is a need to design, fabricate, and characterize these devices. This lab utilizes a wide range of techniques from atomic-scale characterization to reliability testing in switching circuits. This lab provides key correlation of material physics to system performance of power conversion system, including reliability. Key capabilities include MESA fab, defect spectroscopy, electrical characterization, and material and device modeling.
Magnetic Characterization Laboratory 	Magnetic components, including inductors and transformers, provide essential functions such as storage, filtering, galvanic isolation and coupling during the power conversion process. The critical part of a magnetic component is the magnetic core. Current soft magnetic core materials do not meet all the requirements of emerging power electronics that require high switching frequency for increase performances. As such, new magnetic core materials with low loss and high frequency operation needs to be developed and tested. Key capabilities include state of the art materials synthesis (gloveboxes, fume hoods with Schlenk lines, solvothermal reaction vessels, Spark Plasma Sintering), SQUID magnetometry, and B-H analysis up to 10 MHz and 150C.
Advanced Capacitor Laboratory	Like magnetic components, capacitors are also widely used in power conversion systems. They play a key role in power conditioning, filtering, and signal coupling or decoupling. Since they have varying applications, they are widely used in a wide range of industries, including

Facility	Description
	energy storage systems. At the basic level, capacitors store electrical charge utilizing two electrical plates separated by a dielectric material. The dielectric breakdown and aging are of key concerns for highly reliable system requirements. There is a need to understand failure physics for better reliability models to develop next generation capacitor materials. Understanding of reliability and root cause of failures leads to capacitor design changes, circuit-level reliability estimates, and expanded capacitor capabilities. Key capabilities include lab-scale processing for fabrication of next generation dielectrics, and suites of dielectric measurement capabilities for evaluation such as DC HALT, Burn-in, Impedance Spectroscopy, and Q-V curve and C(V) measurements, and more.

3.2.3. Power Electronics Technology – Gaps, Challenges & Needs

A PCS is composed of an inter-related hierarchy of materials, components, and subsystem. This is shown graphically in Figure 10. Improvements in any single layer of the hierarchy can reshape the opportunities in adjacent layers and translate directly to system-level improvements. Conversely, weaknesses in any single layer can dramatically limit the performance of the overall system.

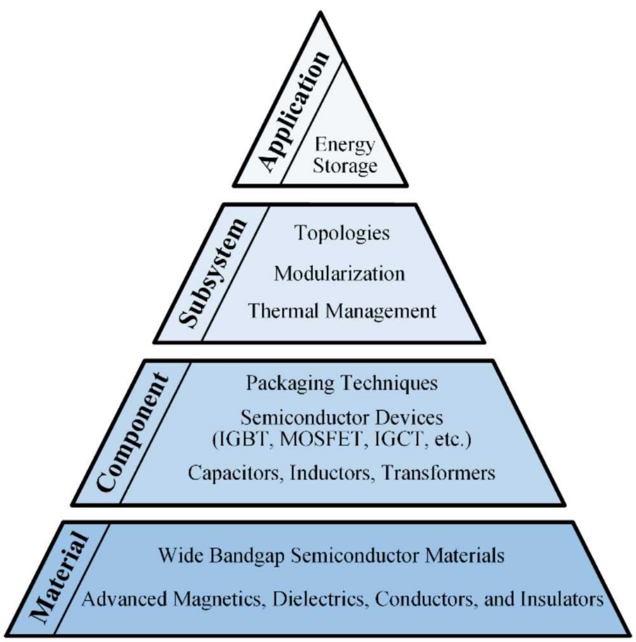


Figure 10. Power Electronics R&D Spectrum

Multiple challenges and research needs exist in each of these layers and some are highlighted in Table 3 below.

Table 3. Examples of PCS challenges and needs for grid storage.

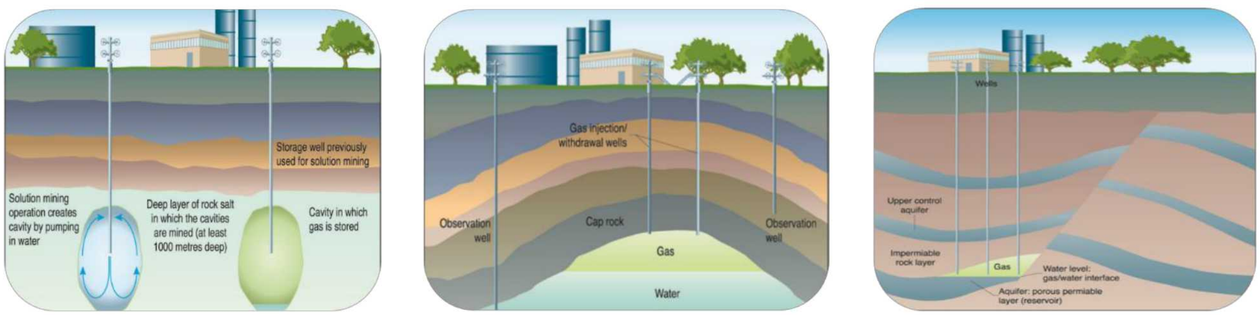
	Challenges	Needs
System	• Disparity between low voltage devices and high voltage grid interface. • Poor DC voltage scalability in converters for electrochemical energy storage systems • PCS are current limited and must be compatible with existing protection schemes	• Isolated DC-DC converters with high DC voltage gain for low voltage energy storage • Advanced modular PCS topologies for energy storage systems • PCS controls schemes that maintain compatibility of legacy protection schemes
Subsystem	• Repairability and serviceability of PCS are required in utility-scale systems • High power density and high temp converters creates more thermal and electrical design restraints • Component susceptibility to thermally induced failure modes	• Modular converter designs consisting of multifunctional power electronics building blocks • New packaging technology for high temp and high voltage operating conditions • High performance active thermal management systems
Component	• High voltage energy storage system interface • High frequency and high temp packaging • Large footprint of inductors and transformers • Capacitors have limited current inrush and temperature limitations • Passive reactance due to discrete components	• High voltage and high-performance post silicon semiconductors • Low inductance packaging and topologies to enable high frequency switching • Innovative magnetic device design such as nanoinductors • Advanced high current, high capacitance, low inductance, and high temp capacitors • Further integration of components to minimize parasitics
Materials	• Gate oxides for semiconductors have a limited temperature range • Magnetic materials suffer from excessive losses at high frequency • Capacitors with low lifetime and limited temp and current ratings • Wide bandgap materials have some limitations in performance	• Reliable next-gen gate oxide material rated greater than 150C • New lower loss magnetic materials that don't suffer magnetization values • High temp, high capacitance, low loss, higher lifetime capacitors • New semiconductor materials having higher voltage, higher thermal ratings with increased availability to decrease cost of substrates

3.3. Subsurface-Based Energy Storage (Stephen Bauer, Org. 8866)

3.3.1. Subsurface Storage Technology – Background

Large-scale subsurface energy storage (both hydrocarbons [oil, natural gas]and non-carbon [hydrogen, air]) can provide means for a better integration of renewable energy sources, balancing supply and demand, increasing energy security, enhancing a better management of the grid and moving the country towards a low carbon economy. Sandia has been involved in site characterization, laboratory and in situ field testing, and complex coupled thermal-mechanical-hydrologic analyses of engineering geologic formations used for subsurface energy storage. Access to the storage is through constructed wellbores; the integrity of wellbores for the life cycle of the underground storage facility is critical to the storage system. Sandia has taken a leadership role in wellbore integrity.

Large containers (~$10^4 – 10^6$ m^3) may be "defined" or constructed underground by using a combination of natural and engineered means and measures. In these containers, liquids and gases may be stored, generally at a pressurized condition (Figure 11).



Salt caverns are solution mined cavities within either **salt domes** or **bedded salts** that do not match reservoir volume capacity.

Depleted reservoirs are proven gas reservoirs that are easy to develop and operate due to existing infrastructure.

Aquifers are similar in geology to depleted reservoirs, but must be proven to trap gas.

Figure 11. Examples of underground storage containers.

The storage space in the containers may be comprised of *rock porosity*, the relatively small space between individual grains, or larger *mined openings* (in the range of 10^6 m^3).

For rock porosity-based storage facilities, geologic barriers (for example stratigraphic or structural) form sufficiently low permeability zones to "prevent" fluid loss. In practice, these storage facilities are often depleted hydrocarbon reservoirs or aquifers that are "strategically" located for their storage purpose. Depleted hydrocarbon reservoirs are the most common underground storage source in the US. Studies have developed relationships between porosity, permeability and well diameter and spacing to evaluate the economics of reservoir storage [7]. Studies have also evaluated the feasibility, fluid mechanics, and safety of converting from hydrocarbon to non-hydrocarbon storage [8, 9].

Mined openings are constructed by "hard rock" mining methods and/or solution mining. Hard rock mines are costly if developed from a green condition and are likely more economic if preexisting at an appropriate depth. Some mines will function as a gas storage container as they exist, (e.g. [10]) and some may require additional engineering measures such as a "water curtain" (e.g. [11]).

Mined openings for storage by solution mining in salt formations take advantage of the low permeability of salt, its ease of mining by solutioning, and creep (and self-healing of cracks) have proven to be wonderful containers. Sandia has been involved in site characterization of domal and bedded salt, lab studies of thermal, mechanical and hydrologic properties since the late 1970's as part of the development of the Strategic Petroleum Reserve (SPR) [12]. The level of sophistication of testing and analysis has matured through the years; Sandia salt mechanics studies are highly regarded worldwide, in part due to our stewardship of the Waste Isolation Pilot Plant, and as geotechnical advisors to the US DOE for the SPR. An example of the sophistication and detail in the analyses is illustrated in Figure 12, where 20 caverns may be simultaneously represented for their time-dependent response to internal fluid pressure changes [13]. This study utilizes ADAGIO, the most recently Sandia-developed 3D solid mechanics code. It is written for parallel computing environments, and its solvers allow for scalable solutions of very large problems. ADAGIO uses the SIERRA Framework, which allows for coupling with other SIERRA mechanics codes.

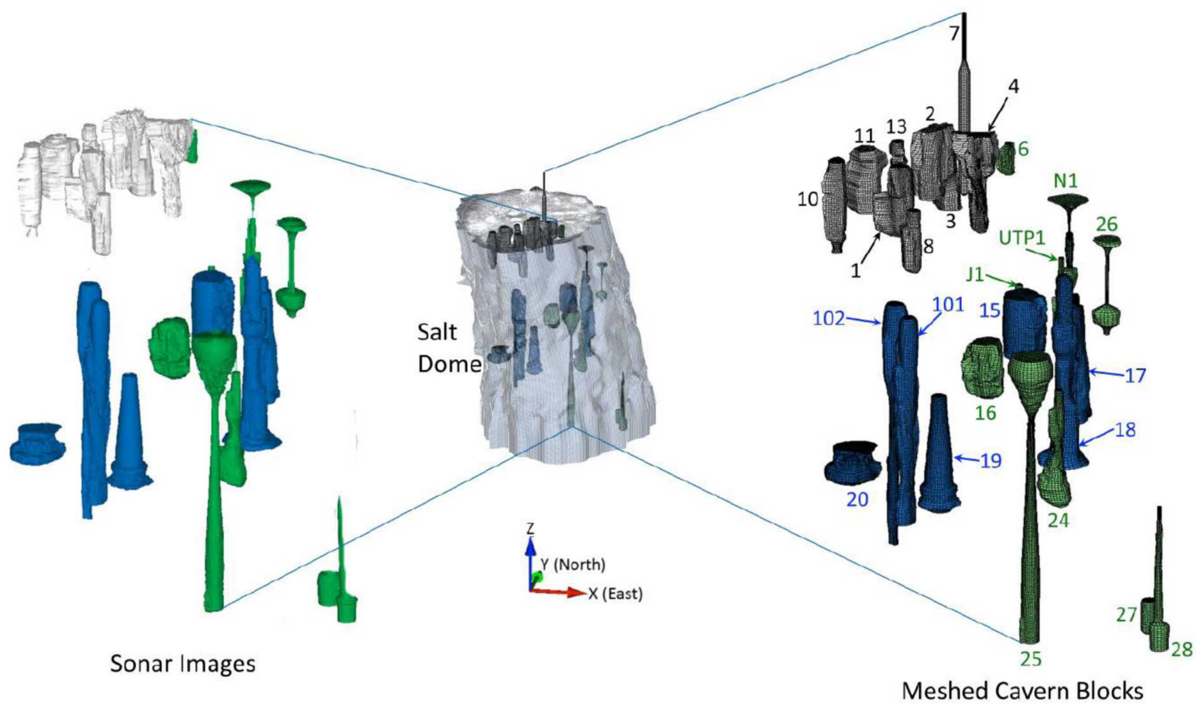


Figure 12. Sonar images (left) and hexahedral finite element meshed block (right) of 26 caverns in the Bayou Choctaw salt dome. The salt dome image is about 2 x 10^3m tall, the caverns range in height from 10^2 to 10^3m, and range in volume from 1 x 10^5m^3 to 3 x 10^6 m^3 [13].

The SPR related studies, utilizing unique characterization/modeling methods, extended to private industry supporting natural gas storage. Sandia helped natural gas industry grow through the Hub concept of storage to take advantage of peak shaving, and accelerated cavern construction though development of solution mining under gas (SMUG). The honest broker approach to natural-gas storage analyses led to characterization and analyses to support the first commercial hydrogen cavern in the US.

Access to the underground is via wells, a constructed component of an underground storage system. Well integrity is ensured through the application of technical, operational and organizational solutions to reduce risk of uncontrolled release of stored fluids throughout the well life cycle. Well integrity has long been part of Sandia's work scope, for the SPR, addressing cavern access to meet mandated deliverability and through the Geothermal related research (e.g. development of PDC cutters). The Macondo oil leak, followed by the Aliso Canyon natural gas leak [14] re-propelled Sandia into well-integrity studies to support national interests. As an extension to these long-standing programs, Sandia has developed a well integrity research thrust area that includes mechanism evaluations (e.g., [15]), materials development (e.g. [16]), materials and system testing at in situ conditions (e.g. [17]), sensing/detection, and life-cycle systems modeling (e.g. [18]).

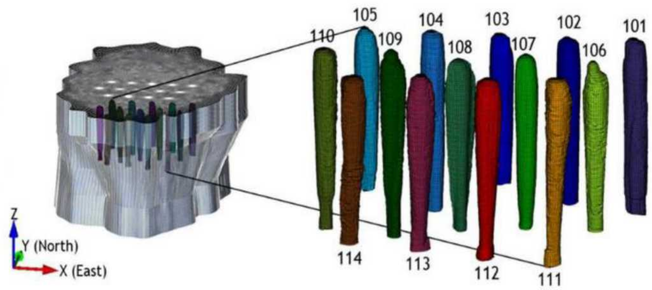
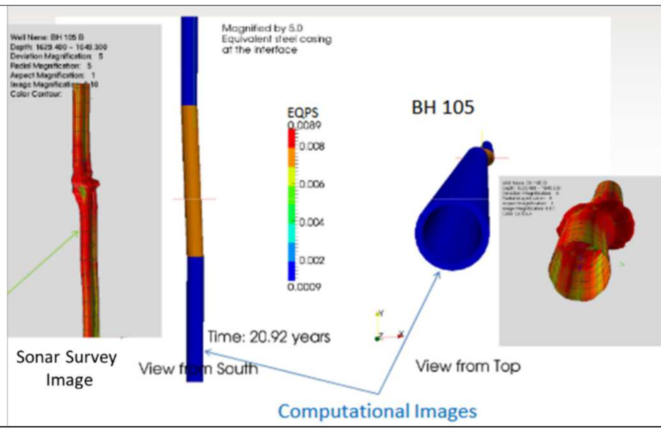
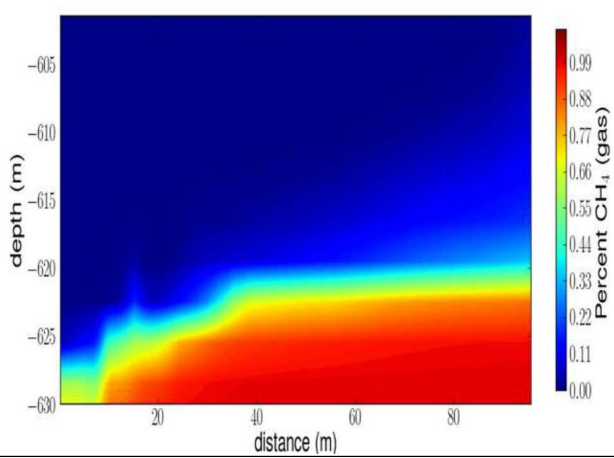
3.3.2. Subsurface Storage Technology – Sandia Capabilities

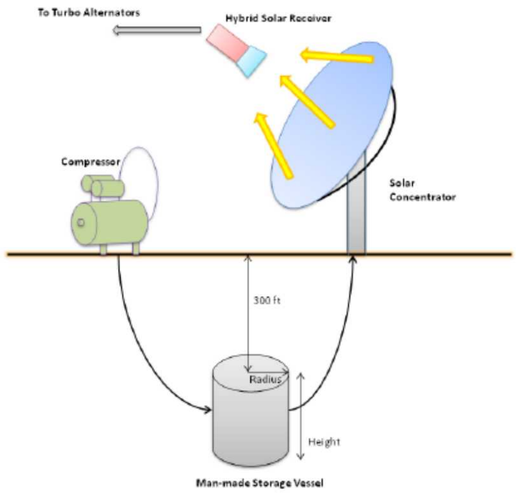
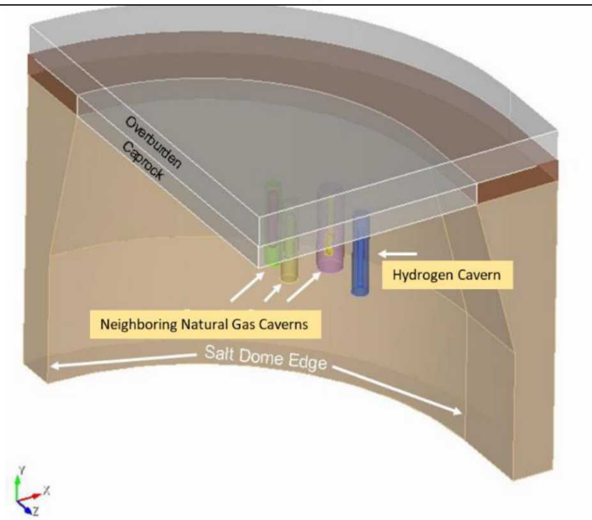
Sandia has been engaged with DOE and Industry partners to characterize, design, model, and test key components of underground energy storage systems (geologic and engineered), and to develop planning/simulation tools to address research challenges and de-risk components and processes. For underground hydrocarbon storage, Sandia is the geotechnical advisor to the DOE for the SPR where 60 aging salt caverns, 120+ wells, and 40+ year old infrastructure must be maintained for its well integrity, cavern integrity, and well design. For natural gas storage, ~12 projects have been studied over the last 20 years resulting in storage of 400 billion cubic feet of natural gas, utilizing state of the art geomechanics testing and 3-D numerical analyses. To support development of compressed air energy storage (CAES), Sandia has completed studies for both DOE and industry-funded projects. These have been in depleted natural gas reservoirs, salt caverns, aquifers (in association with wind), hard rock mines using water curtains in the upper Midwest in conjunction with wind energy [19], in an abandoned limestone mine in conjunction with surplus baseload electric supplies, and buried reinforced concrete vessels (in association with solar). Sandia was engaged to provide the characterization and analysis for the nation's first commercial hydrogen underground storage facility [20] and has assessed hydrogen storage in other lithologies [21].

These projects utilized the DOE's flagship geomechanics laboratory, state-of-the-art 3-D geomechanical modeling capabilities (for example finite element codes such as SIERRA/ADAGIO),[2] and PFLOTRAN, a robust petascale reactive multiphase flow and transport code. Subsurface sensors development, field scale testing and deployment is actively underway. For caverns, small-leach salt-solution mining software has been developed to support small oil movements [22], and a real-time cavern leak monitoring system has been developed and deployed [23, 24]. Underground storage capabilities examples are shown in Table 4.

[2] ADAGIO is the most recently Sandia-developed 3D solid mechanics code. It is written for parallel computing environments, and its solvers allow for scalable solutions of very large problems. ADAGIO uses the SIERRA Framework, which allows for coupling with other SIERRA mechanics codes.

Table 4. Examples of underground energy storage applications

Image	Application Description and References
	Strategic Petroleum Reserve (SPR) consists of 60 aging salt caverns, 120+ wells, 40+ year old infrastructure: well integrity, cavern integrity, well design. Sonar images converted to finite element mesh for geomechanical analysis/simulation of Big Hill SPR site [25].
	Sonar and computational images of wellbore deformation due to differential movement at a geologic interface [26].
	Conversion of Natural Gas Reservoir to Compressed Air Energy Storage. Gas phase composition (CH4 per cent versus depth and distance from the borehole) 100 days after injection began for gas bubble, just before pressure cycling begins [8].

<table>
<tr><th>Image</th><th>Application Description and References</th></tr>
<tr><td>
</td><td>Designed/engineered buried reinforced concrete vessels in association with solar generation [27].</td></tr>
<tr><td>
</td><td>Underground commercial storage of hydrogen in salt cavern. State-of-art analyses simulated cavern pressure conditions during debrining and for proposed future loading cycles. The effects of cavern mining and operations on surface subsidence, storage loss, and cavern stability as a function of time were investigated [20].</td></tr>
</table>

3.3.3. Subsurface Storage Technology – Gaps, Challenges, and Needs

Subsurface-based energy storage technologies represent a large-scale energy storage resource. The conundrum is that not all of the subsurface is readily suitable for storage where the storage is needed; co-location of storage with generation is sometimes problematic. Better and novel ways to engineer the subsurface are required including the following:

- Large subsurface containers that can be created in safe, stable and economic manners essentially anywhere in the US
- Improved excavation technologies
- Technologies to seal volumes of rock at depth into porous "containers" in an analogous manner that geologic processes seal water, oil and gas resources.
- Inclusion of improved degradation, well-integrity, and reliability of subsurface storage systems in geologic and technoeconomic models to improve the design of large-scale, long-duration subsurface storage systems.

Addressing these needs would improve both the flexibility and availability of subsurface energy storage. Sandia could impact the national needs through working with industry to: (1) enhance large scale subsurface excavation technologies, (2) develop means to artificially seal and monitor rock volumes, and (3) develop means to improve underground storage system components.

3.4. Thermal / Thermochemical Energy Storage (Cliff Ho, Org. 8820)

3.4.1. Thermal/Thermochemical Storage Technology – Background

Thermal storage technologies have the potential to provide large capacity, long-duration storage to enable high penetrations of intermittent renewable energy, flexible energy generation for conventional baseload sources, and seasonal energy needs. Thermal storage options include sensible, latent, and thermochemical storage technologies. Sensible thermal storage includes storing heat in liquids such as molten salts and in solids such as concrete blocks, rocks, or sand-like particles. Latent heat storage involves storing heat in a phase-change material that utilizes the large latent heat of phase change during melting of a solid to a liquid. Thermochemical storage converts heat into chemical bonds, which is reversible and beneficial for long-term storage applications.

3.4.2. Thermal/Thermochemical Storage Technology – Sandia Capabilities

Thermal and thermochemical energy storage technologies have been designed, tested, and evaluated at Sandia's National Solar Thermal Test Facility (NSTTF) in Albuquerque, a unique large-scale engineering laboratory and test facility for concentrating solar power (CSP) and solar thermal technologies located several miles southeast of TA-III [28]. The NSTTF includes the following test facilities and capabilities:

- 6 MWth central receiver test facility with 200+ heliostats
- 1 MW_t falling particle receiver system, an engine test facility
- 16 kW_t solar furnace
- High-flux solar simulator (~6 kW_t and ~1 MW/m^2 peak flux) with automated sample handling and exposure system (ASHES)
- Molten salt test loop
- Facilities and equipment for testing CSP components and systems (Figure 1).

For over 40 years, Sandia has been leading R&D in solar thermal energy technologies, including research in power production, thermal energy storage, process heat, thermochemistry, and solar fuels. High-performance computing resources are also available for detailed computational fluid dynamics modeling of complex, coupled processes associated with solar thermal processes. Figure 13 shows the layout of the test facilities at the NSTTF, and Table 5 provides a detailed summary of the various facilities and capabilities at the NSTTF.

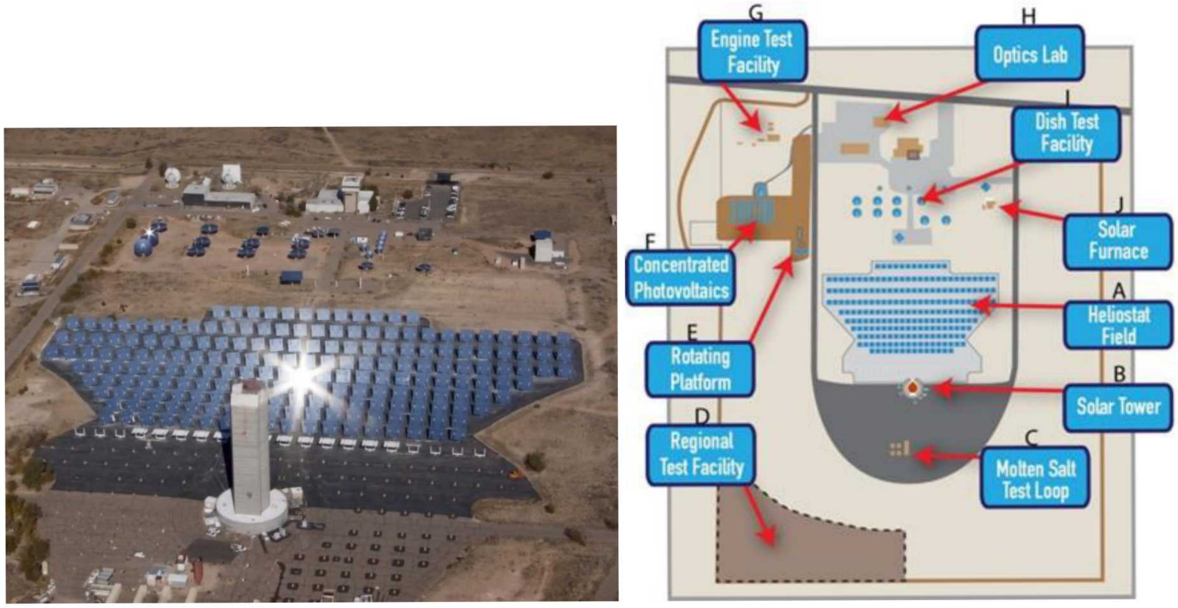
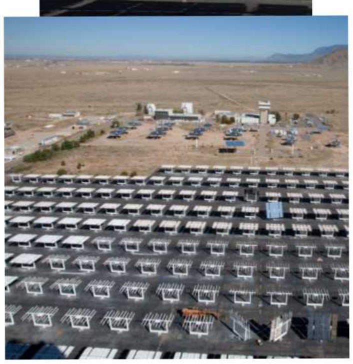
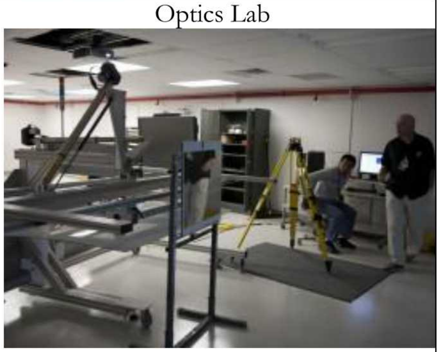
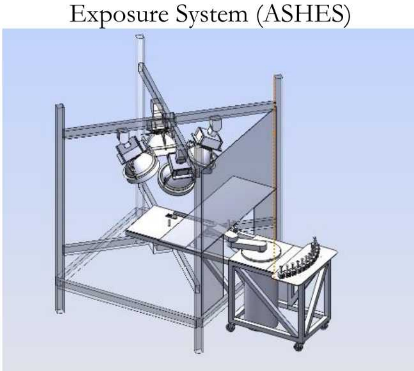
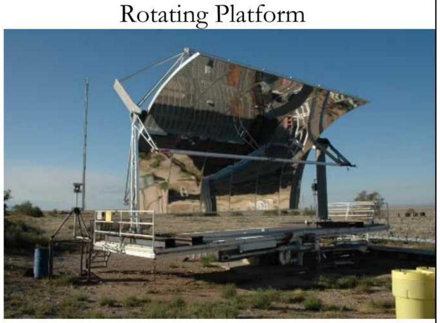


Figure 13. Diagram showing the large-scale test facilities at the NSTTF.

Table 5. Summary of facilities and capabilities at the NSTTF.

Facility	Description
Solar Tower & Heliostat Field  	The tower is a 61 m (200 ft) high concrete structure with three test locations on the north side and the top of the tower. The tower can support testing for CSP experiments and large-scale, high-flux materials samples. The equipment in the tower includes a 100-ton capacity elevating module for lifting experiments to the top of the tower, internal cranes for receiver fabrication, water glycol cooling systems and air coolers to provide heat removal from experiments, air compressors, control valves, generators, uninterruptible power supplies, piping systems, and pressure relief valves. The heliostat field has 218 individual heliostats. This capability can support SunShot projects with prototype scale testing by providing flux levels of greater than 250W/cm^2 and total power in excess of 6 MWt. The capabilities of the helostat field include a thermal capability of 6.0MWth. The solar tower has a target located at the 29m height, and test bays at 37.5m, 42.7m and 48.8m, and on the tower top at the 61m altitude. The tower has an integrated cooling water/glycol system for the cooling of targets under test. The top tower-top flux gage system permits flux measurement for the full power of the field.

Facility	Description
Solar Furnace 	The 16 kW solar furnace has a primary heliostat, a secondary concentrator, and a test table where experiments or calibrations are performed. The peak flux provided is greater than 600 W/cm^2. The furnace is used for selective absorber testing, small-scale receiver testing, and material screening. The furnace has also been used to demonstrate the feasibility of the Sunshine-to-Petrol initiative.
Optics Lab 	Optical equipment located in this lab space and tools developed, using DOE funds, allows for detailed optical characterization of heliostat, trough and dish facets. These flexible analytical tools, along with the on-site expertise currently support the evaluation and development of low-cost, high-performance heliostat facets. In addition, field support for characterization and alignment of CSP systems is provided. SOFAST, a highly accurate fringe-reflection-based measurement tool, is used to characterize and set the focus heliostat facets in the laboratory at sizes to 6x12 feet. H-FACET is an optical-based alignment tool that is used to efficiently re-align the facets after re-attaching them to the heliostat. AIMFAST is used to characterize dish facets and align dish systems.
High Flux Solar Simulator with Automated Sample Handling & Exposure System (ASHES) 	A high-flux solar simulator with automated sample handling & exposure system (ASHES) has been developed to rapidly expose multiple samples to simulated concentrated sunlight and high temperatures. ASHES provides accelerated lifetime-aging tests of materials under high-temperature/high-flux conditions. A robotic sample handling system automatically moves coupons into and out of the concentrated flux sequentially to expose multiple samples to predetermined temperatures, fluxes, and/or durations. The high-flux simulator consists of four 1800 W metal-halide lamp. The total emitted radiative power is 1500 W per lamp (6000 W total) with a peak irradiance of ~1.1 MW/m^2 and an average irradiance of ~0.9 MW/m^2 over a spot size of ~1 inch (2.5 cm). The lamps and elliptical reflectors are arranged in a beam-down configuration to provide ease of sample handling and exposure on a horizontal surface beneath the lamps.
NSTTF Machine Shop & Assembly Facility	A small but capable machine shop including basic heavy equipment such as lathes, drill presses, sanding stations, band saws, welding operations, overhead crane, and other basic shop equipment is available on site. The equipment and technicians are capable of hermetic welding of high-tech alloys including Haynes-230 and Inconel 600-series alloys. A 2500 ft^2 building and has a 34 ft ceiling and a 5-ton mobile crane with a 24 ft lift. Welding tools and the capability of welding exotic materials with high nickel content (such as Haines 230 and the Inconels) is housed here. An adjoining machine shop with lathes, mills, band saws, etc. is present. Staff associated with this facility has decades of experience with assembly of solar-tested components and cooling systems for a high flux environment.

Facility	Description
Molten Salt Loop (MSTL) 	The MSTL system at Sandia National Laboratories is a unique facility for the testing of solar components and on-sun collectors in molten flowing nitrate salt in realistic plant-like conditions. MSTL provides 3 parallel test loops for customers to evaluate components in salt service. The system can provide flowing salt at 400-600gpm (depending on temperature), 300-580°C, and pressure to 600psi. The system has a 1.4MWth air cooler to remove heat from on-sun testing of CSP collector systems. This system is the largest flowing salt system available for customer testing of components and on-sun collectors in the world.
Molten Salt Compatibility Test Vessels	Molten Salt Compatibility Test Vessels are used by Sandia for long-term evaluation of salt corrosion mechanisms, materials compatibility, and electrochemical work. The items, contained in 2 facilities, include 700°C salt vessels for 3000hr tests of 32 coupons per vessel. The second design is of smaller capacity (~0.5kg salt), but is able to achieve nearly 800°C, with a gas overpressure, and also has an interchangeable liner. This vessel is also instrumented with mass spectroscopic capabilities to allow analysis of the ullage space over time, which would allow determination of possible off gas products. In addition, this vessel will be used for the electrochemical work including corrosion testing at high temperature.
Rotating Platform 	Outdoor 10'x 20' platform rotates 360 degrees under computer control. Used to test components under specific solar angles of incidence. Complete data acquisition systems.
Component Test Facility	Features an assembly bay, two test cells, control room, and bench test capabilities. Each bay has a variety of energy supply options. An Eddy Current Dynamometer is available for engine testing, and an external cooling system is available. A large furnace is available for testing components under high temperature conditions (up to ~800 °C).
Dish test facility	Dish systems of 41 and 80 square meters are available for on-sun testing. Each is capable of peak concentration over 10,000 suns, and delivers highly characterized beam profiles to customer packages. Supportive optical modeling is available to predict flux profiles on shaped packages. Significant refurbishment would be required to get the dish test facility back up and running.

Facility	Description
Software and Computational Fluid Dynamics Modeling	Sandia and the NSTTF maintains a full suite of software needed for engineering design, analysis, data collection, control, and evaluation including SolidWorks (with fluid, heat, and mechanical FEA), FLUENT, MATLAB, LabView, and others.

3.4.3. Thermal/Thermochemical Storage Technology –Gaps, Challenges, and Needs

The relatively low energy density of sensible-heat storage materials requires large volumes for large-capacity energy storage, which increases the overall storage cost. In addition, some power cycles that employ recuperation to increase the thermal-to-electric efficiency require relatively low temperature differentials between the hot and cold states of the storage media. For example, the supercritical CO_2 recompression Brayton cycle requires a temperature increase of only ~200 °C in the primary heat exchanger [29]. As a result, the required mass inventory of storage material must increase to deliver the same amount of energy with a lower temperature differential, which increases costs. The target capital cost for the DOE CSP program is $15/kWh for the entire thermal storage system. Molten salts freeze at >200 °C, which requires expensive trace heating to maintain all components at temperatures well above the freezing point. If the salt freezes, flow can be blocked, and thawing must occur before operation can begin. Stress within the large storage tanks has also caused issues at CSP plants. Thermal gradients at the base of the tank can create thermomechanical stresses that damage the tank structure. Appropriate consideration of thermomechanical stresses is critical to the design of large-scale thermal storage tanks. Additional research and capabilities are needed in the area of heat exchangers, low-cost, robust materials with desired thermophysical properties, and improved designs for low-cost, highly insulating, large-scale storage systems for large-capacity, long-duration storage (>GWh).

Challenges with phase-change materials (PCMs) include relatively high costs and narrow operating temperature ranges. Using PCMs to provide energy to a heat engine will typically require a cascaded system with multiple PCMs with different melting points. The use of molten silicon at high temperatures provides challenges with materials containment and heat loss. Phase-change systems must still be well insulated to prevent heat loss and subsequent phase change. Additional research and capabilities are needed in the area of materials to increase latent energy storage and improve containment at low costs.

While the concept of thermochemical energy storage holds much promise, multiple challenges exist before the technology is ready for prime time. Overarching issues include (1) development of novel solar receiver and reactor configurations that can be integrated into CSP designs; (2) low heat transfer efficiencies; (3) lack of large-scale testing and data; (4) material cyclability and lifetime; and (5) comprehensive technoeconomic analyses to determine cost, viability, and impacts. However, these challenges are not insurmountable, and ongoing research efforts can address the shortcomings. In addition, Sandia's National Solar Thermal Test Facility is well-suited to address these challenges.

3.5. Hydrogen Storage (Jonathan Zimmerman, Org. 8367)

3.5.1. Hydrogen Storage Technology – Background

Widespread use of hydrogen as an energy carrier and alternative fuel has the potential to impact transportation, portable power and stationary power, to improve the nation's energy security through reduction in fossil fuel dependency, to reduce carbon dioxide and other greenhouse gas emissions, and to enhance electric grid resiliency [30, 31]. Much of this potential relies on the use of polymer electrolyte membrane (PEM) fuel cells, which convert pure hydrogen into electrical energy. Hydrogen has the highest energy per mass of any fuel; however, its low ambient temperature density results in a low energy per unit volume. This aspect of hydrogen necessitates the development of advanced storage methods that have potential for higher energy density, especially for on-board use in transportation and other applications involving portable power [31].

Storage of hydrogen can be accomplished in several ways. For transportation, fuel cell electric vehicles (FCEVs) have been developed and made commercially available. On-board storage of hydrogen is done using carbon fiber-reinforced composite tanks capable of storing the gas at room temperature with a fill pressure of either 350 or 700 bar (~5076 or 10153 psi), depending on the vehicle's design and desired driving range [30]. To facilitate fueling of these vehicles, hydrogen stations have been concurrently designed and constructed to store large amounts of hydrogen (~300-600 kg/day) on-site in its liquid form. In their current construction, these stations rely on compression and pre-cooling technologies that add complexity to the fueling process and introduce penalties with regard to cost, reliability, durability, and energy consumption. Pressure vessels for fueling infrastructure (and other applications where large amounts of hydrogen are used) typically consist of steel alloys of nickel, chrome and molybdenum, which maintain adequate structural properties upon exposure to hydrogen at cryogenic temperatures.

The U.S. Department of Energy (DOE), in conjunction with U.S. DRIVE (Driving Research and Innovation for Vehicle Efficiency and Energy), a public–private partnership between DOE and automotive, energy, and utility companies, has developed hydrogen storage system targets for light-duty FCEVs [31-34]. These targets include fueling system gravimetric capacity, system volumetric capacity, and cost per energy unit, and are shown below in Table 6, adapted from reference [30].

Table 6. U.S. Department of Energy onboard hydrogen storage targets compared to the performance of 700 bar compressed storage technology. (adapted from reference [30])

	700 bar compressed gas (2018)	2020	2025	Ultimate
Fueling system gravimetric capacity [wt% H2]	4.2	4.5	5.5	6.5
Fueling system volumetric capacity [g/L H2]	24	30	40	50
Cost [$/kW-hr]	15	10	9	8

As noted in reference [30], these values pertain to the entire storage system, including both the tank and associated balance-of- plant (BOP) components. It is physically impossible to meet the 2025 and ultimate volumetric capacity target with pressurized gas at room temperature, as the density of hydrogen gas at 700 bar is just 40 g/L without accounting for any additional system inefficiencies. DOE has determined that these targets also apply for class 8 long-haul fuel cell electric trucks [32-34], technology still under development in the U.S.

An alternative method for storing hydrogen is within a solid material, stored as individual atoms within the solid's molecular structure. Complex metal hydrides possess both large gravimetric and volumetric hydrogen densities, up to 15 wt% and over 100 kg m^{-3}, but face challenges such as sluggish kinetics at low temperatures and the formation of stable intermediate phases that reduce the capacity over time [35]. Current strategies are focused on methods such as nanostructuring to facilitate improvements in these areas [36], among other routes being pursued. Another solid-storage option, porous adsorbents, have the potential to offer rapid filling times and delivery response, long cycle life, and easily controlled delivery pressures, but also have limitations of their volumetric and gravimetric capacities [30].

Research on hydrogen storage at Sandia is focused in two areas: (1) Characterizing and understanding the physical limitations of solid-storage materials to enable the development of novel materials that can go beyond these property and performance limits, and (2) Developing a deep understanding of the composition-processing-microstructure-property relationships for metal alloys used in hydrogen infrastructure components such as pressure vessels to guide materials selection and alloy development at the industrial scale. For area (1), Sandia maintains extensive facilities for the design, synthesis and characterization of hydrogen storage materials and has a team of experts to solve important technical problems in this area of research [37]. Staff at Sandia have been researching hydrogen storage materials that can release hydrogen gas with very little energy input, and that also can rapidly take on hydrogen during re-fueling at a hydrogen filling station. Major hydrogen solid-storage research activities include:

- Fundamental studies of hydrogen interactions with solid-state materials;
- Design and synthesis of promising on-board reversible hydrogen storage materials with exothermic hydrogenation and appropriate kinetics and cycling behavior;
- Understanding processing-structure-property relationships for improved materials performance through compositional, structural, catalytic, and nanostructure modification;
- Developing *in situ* techniques to characterize hydrogen storage materials and elucidate the role of intermediates, defects and interfaces on hydrogen diffusion and reaction pathways;
- Engineering and process development to accelerate the transition of the best hydrogen storage materials to a commercial reality.

Research in area (2) constitutes a portion of a broader scope of activities surrounding compatibility of materials with hydrogen [38]. Materials compatibility research at Sandia examines the response of structural (e.g. austenitic stainless steels, ferritic pipeline and pressure vessel steels, aluminum alloys) and functional (e.g. polymers) materials used ubiquitously in both FCEVs, fueling infrastructure, and other industrial applications of hydrogen. The DOE Hydrogen and Fuel Cell Technologies Office (HFCTO) has designated Sandia's hydrogen-materials compatibility capability as "core" for their program, a unique laboratory contribution that they expect us to lead for the nation.

Sandia co-leads several multi-lab consortia for DOE that draws equally upon our hydrogen and materials science capabilities and knowledge, namely H-Mat (hydrogen-materials compatibility), HyMARC (solid state hydrogen storage materials), and HydroGEN (solar thermo-chemical hydrogen production materials). These consortia focus on developing a fundamental understanding of the underlying phenomena and processing-structure-property relationships that limit the properties for their respective materials of interest, and in devising materials discovery strategies to meet DOE property and performance targets.

3.5.2. Hydrogen Storage Technology – Sandia Capabilities

Capabilities at Sandia are rooted in interdisciplinary research that enables self-assembled materials, tailored alloys, multicomponent composites, destabilized and nanostructured metal hydrides to be conceived, synthesized, characterized and evaluated for vehicular hydrogen storage. Staff expertise ranges from solid-state physics, surface chemistry, materials theory, simulation, design, and synthesis to using state-of-the-art instruments to evaluate materials performance under various process parameters and extreme environments. Phase equilibrium codes using a large thermochemical hydride database developed by Sandia are used to predict the plateau hydrogen pressure and concentration of all relevant species at equilibrium. State-of-the-art experimental capabilities available at Sandia and through our technical collaborations include:

- Numerous gloveboxes and Schlenk lines
- High-pressure reactor stations (>2000 bar H_2 pressure)
- PCT and Sieverts instruments
- *In situ* X-Ray and neutron diffraction (XRD, ND)
- Electron microscopy techniques such as Scanning Electron Microscopy. (SEM), Scanning Tunneling Microscopy (STM), and Transmission Electron Microscopy (TEM)
- Environmental & ultra-high vacuum X-Ray Photoelectron Spectrometery (e-XPS and XPS)
- In situ Differential Scanning Calorimetry (DSC) systems
- Thermo-Gravimetric Analysis and DSC (TGA-DSC)
- Nuclear Magnetic Resonance (NMR)
- Synchrotron-based soft-x-ray emission & absorption spectroscopies, via partnering facilities such as the Advanced Light Source at LBNL and the Stanford Linear Accelerator Center.

Several of these capabilities are shown in Figure 14.

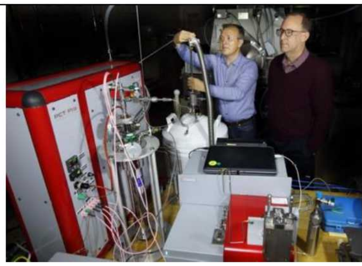
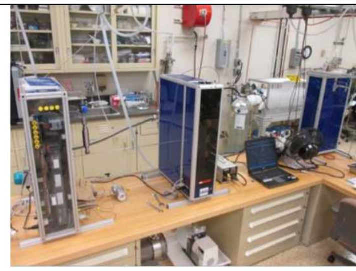
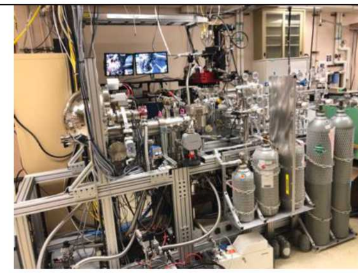
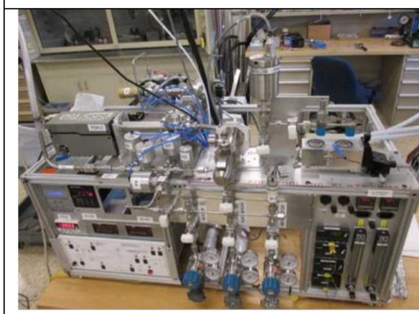
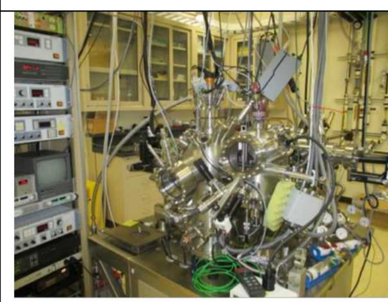
		
PCT-Pro instrument	PCT & Sieverts instruments	Environmental XPS (e-XPS)
		
In situ DSC/RGA system	In situ TGA/DSC/Mass-spectrometry	Ultra-high-pressure reactor
		
Nitrogen glovebox	Argon glovebox	SEM/EDX spectroscopy
		
Low-pressure porosimetry	High-pressure porosimetry	Variable-temperature STM

Figure 14. Scientific research capabilities used to examine materials for solid storage of hydrogen.

For research in hydrogen-materials compatibility, Sandia maintains unique, state-of-the-art research facilities to address both fundamental scientific and applied engineering questions related to the interactions of gaseous hydrogen with materials. Descriptions of these facilities can be found in Table 7.

Table 7. Summary of facilities and capabilities for hydrogen-materials compatibility research.

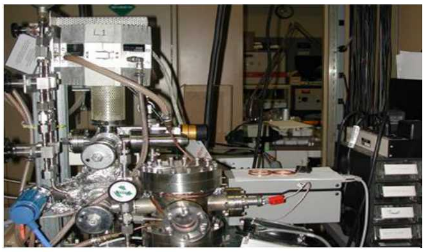
<table>
<tr><th>Facility</th><th>Description</th></tr>
<tr>
<td>Hydrogen Effects on Materials Laboratory
</td>
<td>The Hydrogen Effects on Materials Laboratory is the cornerstone of Sandia's research expertise in hydrogen compatibility of materials and a core capability stewarded by EERE's Hydrogen and Fuel Cell Technologies Office at the U.S. DOE. The laboratory houses specialized assets for evaluating materials performance in high-pressure gaseous hydrogen.

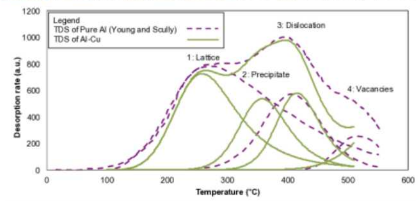
Fracture and fatigue testing in high-pressure gaseous hydrogen – Standard tensile, fracture and fatigue test configurations are executed with concurrent gaseous hydrogen exposure at pressure up to 140 MPa.
High-pressure fracture and fatigue testing at temperature – New capability enables loading of a variety of test specimen configurations (standard tensile, fracture and fatigue tests) at controlled (constant) temperature in the range of 220K to 450K concurrent with gaseous hydrogen exposure at pressure up to 140 MPa.
Constant-displacement, environmentally-assisted crack growth testing – Instrumented fracture mechanics specimens are loaded to constant displacement and exposed to gaseous hydrogen at pressure up to 200 MPa. The temperature can be independently controlled (usually constant) in the range of 200K to 440K. Subcritical cracking threshold and crack velocity can be measured.
Pressure cycling in controlled temperature – New capability allows exposure of non-metals (and metals) to pressure cycles up to 100 MPa at controlled (constant) temperature within the range 220K and 400K.
Thermal precharging – Materials and test specimens are exposed to high-pressure gaseous hydrogen or deuterium (up to 140 MPa) at elevated temperature (up to 300°C) to produce controlled hydrogen content within the specimens prior to evaluation.

</td>
</tr>
</table>

<table>
<tr><th>Facility</th><th>Description</th></tr>
<tr><td>

Hydrogen Transport and Trapping Laboratory





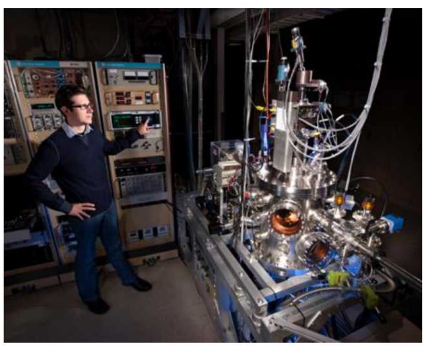
</td><td>

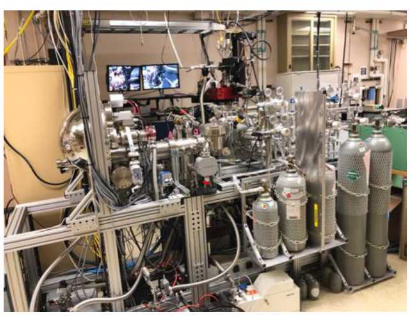
Hydrogen transport and trapping determines many features of the interactions between hydrogen and materials. In particular, the effects of hydrogen on mechanical properties can be strongly influenced by transport (or diffusion) of hydrogen in materials on the time scale of testing.

- ***Gas-phase permeation*** – Permeation and diffusion of hydrogen are measured in two instruments by exposing one side of a thin foil to deuterium at ~0.5 bar and measuring the deuterium molecules that evolve on the down-stream side of the foil, which is at ultra-high vacuum. These tests may be conducted at up to 1000˚C.
- ***Thermal desorption spectroscopy (TDS)*** – A gas-charged specimen is heated at a controlled heating rate to release the hydrogen, which is measured as a function of temperature. The resulting spectrum is analyzed to determine the amount of hydrogen in the material and characterize the "strength" of its interactions with microstructural features.

</td></tr>
<tr><td>

Hydrogen-Surface Interactions Laboratory





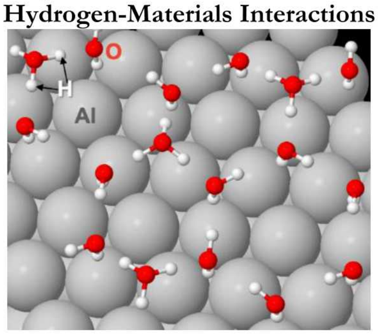
</td><td>

A formidable obstacle to our understanding of hydrogen-surface interactions lack of experimental surface science tools capable of directly detecting hydrogen. To address this gap, Sandia has developed an array of specialized capabilities that can be brought to bear on the problem. The first of these is an angle-resolved ion energy spectrometer (ARIES) for low energy ion beam analysis. This instrument was developed specifically for detection of light adsorbates such as hydrogen and uses low energy ion beams (< 3 keV) to probe the surface. Scattered and recoiled particles then provide information on surface structure and composition; detection of hydrogen concentrations as low as 0.03 monolayers is possible.

Other advanced surface techniques under development address the long-standing problem of how to extrapolate experiments performed in ultra-high vacuum environments to more relevant high-pressure regimes. To bridge this gap, we have developed an ambient pressure or environmental x-ray photoelectron spectroscopy (AP-XPS) and infrared absorption spectroscopy systems (IRAS) to system capable of operating at near-ambient pressures (~10 Torr.) Other advanced techniques such as Kelvin probe force microscopy and electron energy loss spectroscopy are also being exploited to study hydrogen on surfaces.

</td></tr>
<tr><td>

Computational Materials Science of Hydrogen-Materials Interactions

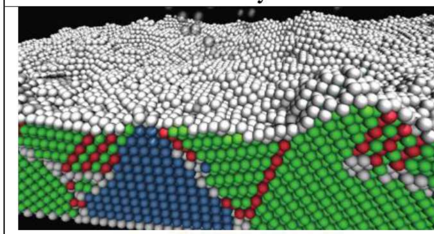
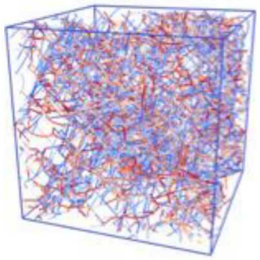


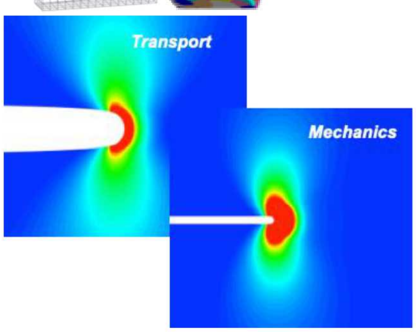
</td><td>

Challenges associated with experimental characterization of atomic scale hydrogen interactions necessitates the use of computational tools to inform the development of predictive models of hydrogen-assisted fatigue and fracture. Robust models must capture the hydrogen-surface interactions and hydrogen transport as well as the mechanisms of hydrogen interactions with microstructural features in the bulk, such as vacancies, dislocations, and grain boundaries. Sandia researchers model hydrogen interactions across multiple length scales, working closely with experimentalists to inform the macroscopic response of materials in hydrogen environments.

- ***Density Functional Theory (DFT)*** – In DFT, the equations of quantum mechanics governing the behavior of electron orbitals are solved to compute the energetics and dynamics of atomic systems with

</td></tr>
</table>

<table>
<tr><th>Facility</th><th>Description</th></tr>
<tr><td>





</td><td>
very high fidelity. This approach provides fundamental insight into the atomistic details of hydrogen's interactions in a material.

Molecular Dynamics (MD) – While DFT is a very accurate approach, its computational cost prohibits studies to a few hundred atoms. With MD, the interactions of millions of atoms can be studied over nanosecond time scales. MD provides a valuable tool for studying fundamental hydrogen-defect interactions (e.g. dislocations, grain boundaries).
Dislocation Dynamics (DD) – A key feature of hydrogen embrittlement is the impact of hydrogen on plastic deformation. DD is a tool where the motion of large ensembles of dislocation lines—crystalline defects whose motion induces plastic deformation—is simulated. The time and length scale of DD allows for a stronger comparison with experiments than possible with MD or DFT.
Crystal Plasticity (CP) – DD simulations are typically limited to single crystals. In contrast, CP is a tool for studying polycrystalline materials, where the response of ensembles of grains is simulated. Direct comparisons with high resolution strain mapping experiments is possible.
Continuum Finite Element Methods (FEM) – Continuum FEM models are the work horse of engineering system design. Multiphysics tools have been developed at Sandia for studying coupled deformation and hydrogen diffusion. Multiscale methods allow concurrent coupling between continuum models and high-resolution models (e.g., CP) in key regions of interest, such as a crack tip.

.
</td></tr>
</table>

3.5.3. Hydrogen Storage Technology – Gaps, Challenges, and Needs

Research performed at Sandia, with its many partners and collaborators, has done much to elucidate the mechanisms that dictate how quickly hydrogen is adsorbed and desorbed from a solid material. Efforts on solid-storage materials have provided an enhanced understanding on how aspects of material bonding and microstructure interact with thermodynamics and kinetics to yield behaviors that bring us closer to performance targets [30, 35, 36, 39-43]. However, knowledge gaps still exist in identifying and validating the combinations of composition, structure, additives and catalysts that will produce materials that rival if not surpass the compressed gas option with regards to both technical performance and affordability. Specific challenges include:

Methods for accelerating materials evaluation and discovery: Much of Sandia's research to-date has built on its past experience in metal hydrides and sorbents, investigating the underlying physics that introduce property and performance limitations for familiar material systems (e.g. Mg-B, Li-N). This research has been vital for identifying key characteristics that can be used to evaluate a material's suitability as a storage medium. Also needed, however, are methods to explore the variations of composition and material structures and evaluate those metrics in a rapid way that considers combinations that are non-intuitive to the experienced researcher.

Two such methodologies present themselves as viable pathways to address this challenge: machine learning (ML) and high-throughput synthesis and characterization. Machine learning algorithms analyze data collected through both experimentation and *ab initio*-based numerical computation to elucidate the relationships between important material properties and atomic and molecular structure-based metrics (descriptors). These descriptors can in turn be used to rapidly screen vast permutations of composition. Sandia has had recent success in developing and applying ML-based techniques, uncovering the strong dependence of the metal hydride equilibrium H_2 pressure on a volume-based descriptor that can be computed from just the elemental composition of the intermetallic alloy [44]. This research has just begun, and other material classes are being examined, such high entropy alloys.

Success with machine learning relies on a large amount of data upon which its algorithms can "train" to determine the relationships between properties and characteristics. Ideally, this data would come solely from experimentation to provide information under 'real world' conditions, e.g. finite temperature, pressure, defect content. However, it's often the case that an insufficient amount of data exists upon which to create a statistically representative model of a material. This lack of data is frequently compensated-for through the use of numerical simulation (e.g. calculations of thermodynamic properties from density functional theory), but an alternative solution is use of high-throughput synthesis and characterization, i.e. rapid creation of a large variety of compounds and measuring their properties in succession. High-throughput experimentation can itself be used as a tool for discovery independent of machine learning, but together the two can be leveraged to make even faster and bolder progress.

Techniques and an underlying knowledge base for low-cost, high-yield fabrication: Scientific research commonly occurs at the laboratory scale, evaluating grams-to-mg of material to isolate characteristics and properties that reveal the promise of target-meeting performance. Discovery of a material that fulfills this promise must go hand-in-hand with the development of methods to fabricate kg-to-ton amounts of that material and do so in a simple and economically efficient way such that it can be embraced as a solution by the hydrogen fuel industry. This challenge will require the deep understanding of how specific processing methods (e.g. ball milling) affect both material structure and integrity. Key to advances in this area will be effective partnerships that integrate Sandia's knowledge of materials with the technical proficiency of both private companies that routinely develop functional materials at similar scales, and other national laboratories that have expertise in devising manufacturing techniques to addressed specialized, as-produced requirements.

Engineered systems that maintain lab-scale performance of discovered materials: Success in both materials discovery and high-yield fabrication is still insufficient to provide a materials-based fueling system that will displace compressed gas tanks. Inefficiencies in hydrogen adsorption and desorption, storage capacity and reversibility may still occur due to aspects of an engineered system such as imperfect thermal transport and insulation, material wear and the presence of impurities introduced through manufacturing and assembly. Modeling, simulation and systems analysis will be needed to explore variations in design and prediction of the impact of these aspects on the system's performance. In addition, recent analysis has been done that demonstrates how aspects of an engineered system introduce trade-offs in a materials ability to meet all of the desired performance targets. In this analysis, finite element analysis of a tank design utilizing nanoscale metal hydrides revealed that significant progress in gravimetric and volumetric capacity is achieved at the cost of lower reversible capacity. This example shows the value that systems analysis can provide in quantifying expectations for real material performance and in enabling co-optimization of the material and the fueling system.

Gaps and research challenges also exist for hydrogen-materials compatibility, and the development low-cost structural alloys used for pressure vessels that store gaseous or liquid hydrogen. The Ni-Cr-Mo steel alloys mentioned earlier have the observed property that the best performance in hydrogen (e.g. highest fracture resistance) is found in alloys with low tensile strengths. Research to-date has revealed a tensile strength threshold at about 950 MPa, above which alloys display a remarkable reduction in fracture resistance from 50-60 MPa-$m^{1/2}$ to 20-30 MPa-$m^{1/2}$. This limitation results in more material needed to meet specific containment requirements, and thus a higher cost for such components. Sandia – through the aforementioned H-Mat consortium – is working to identify processing routes that result in microstructures capable of both high strength and fracture resistance. Nano- and micro-scale modeling is examining features of these microstructures to determine which type of deformation-induced defects can lead to maximized values of both properties. The determination of these processing-structure-property relationships, in both a deterministic and statistical sense, remains a large challenge in developing the best-performing materials. In addition, investigations of compositional variants are also warranted to minimize the content of higher-cost elements (e.g. Ni) in favor of lower cost alternatives that produce the same levels of properties in hydrogen environments.

These represent just some of challenges present in hydrogen storage research, and a desired future state where Sandia is providing insight and solutions for end-to-end development of materials solutions: from formulation to fabrication to application. To achieve this future state and maintain leadership in hydrogen storage, Sandia needs to develop the following capabilities:

- Expertise in application of machine learning methods to materials property optimization
- Equipment for high-throughput materials synthesis and characterization
- Scientific instruments to characterize catalytic materials for liquid hydrogen carriers
- Expanded expertise and modernized lab facilities for synthetic chemistry
- System engineering and modeling expertise for technology development (e.g. solid storage-based fuel tanks)
- Expertise in multiscale modeling and simulation to link microstructure features to engineering scale performance
- Expansion of capabilities for high-pressure materials testing to reach liquid hydrogen temperatures
- Scientific instruments to characterize deformation and microstructure evolution in a hydrogen gas environment

3.6. Data Analytics, Systems Optimization, and Controls (Ray Byrne, Org. 8813)

3.6.1. Data Analytics, Systems Optimization, and Controls - Background

Energy storage is capable of providing a number of grid benefits [45, 46], which are typically categorized based on the time scale. On a slower timescale are energy supply interactions, where large amounts of energy are supplied or pulled from the grid. These are often referred to as "energy" applications. Examples include renewable energy time shift and energy arbitrage in market areas. On the other hand, "power" applications normally transpire on a much faster time scale and are employed to support real-time control of the electric power grid. Examples include voltage support and small signal stability. A summary of grid benefits, divided into energy and power applications, is summarized in Table 8.

Table 8. Summary of Energy Storage Applications.

Energy Applications	Power Applications
Arbitrage	Frequency regulation
Renewable energy time shift	Voltage support
Demand charge reduction	Small signal stability
Time-of-use charge reduction	Frequency droop
T&D upgrade deferral	Synthetic inertia
Grid resiliency	Renewable capacity firming
Capacity	

Quantifying the value of energy storage can be a daunting task. First, the remuneration method is highly location specific. In market areas, energy storage is only compensated when providing services for which there are market products. The locational marginal price (LMP) for many grid services (e.g., energy and ancillary services) can vary significantly from location to location because of congestion as well as zonal pricing. Many markets have rules which limit the ability of energy storage to participate (e.g., by defining minimum discharge times or specifically prohibiting providing multiple services). Market rules also vary under each independent system operator (ISO). In a vertically integrated utility, the value of storage is often tied to the cost savings achieved by deploying energy storage. Production cost modeling is used to quantify the benefit of energy storage to a vertically integrated utility for services that transpire over a slower time scale. For services related to grid stability, like frequency control, dynamic simulation must be performed to quantify the grid benefit of different storage scenarios (e.g., frequency nadir after a large contingency). Because of these factors, the valuation of energy storage is highly location specific.

The siting, sizing, and operation of an energy storage system contribute to the value of the energy storage system. As mentioned previously, the valuation is highly location specific. In addition, an energy storage system must charge and discharge at the correct times to capture the maximum grid value. In the case of reduced demand charges, missing the coincident peak load hours can result in the loss of a significant amount of potential revenue. Therefore, the design of the dispatch control system is critical to successful operation of an energy storage system. At slower time scales the operation can be formulated as an optimization problem. At faster time scales, custom control algorithms are often required. A good example is small signal stability, which requires feedback from multiple locations in the grid and a complex control law to damp multiple oscillatory modes simultaneously.

3.6.2. Data Analytics, Systems Optimization, and Controls – Sandia Capabilities

Sandia has extensive capabilities with respect to energy storage data analytics, system optimization, and controls. Sandia has the following capabilities:

- Extensive project analysis expertise from supporting the Sandia energy storage demonstration program
- QuEST – an open source Python tool for valuing energy storage in market areas and behind-the-meter applications
- EGRET/Prescient – open source Python tools for stochastic production cost modeling, can be used to value energy storage in vertically integrated utilities or for resilience applications
- Extensive experience developing dynamic models with exergy storage scenarios (e.g., PSLF)
- Algorithms for wide area control of energy storage (e.g., optimal fixed structure control), distributed control of energy storage, and optimal dispatch to maximize revenue or grid benefit

3.6.3. Data Analytics, Systems Optimization, and Controls – Gaps, Challenges, and Needs

There are still significant gaps and needs with respect to energy storage modeling. These gaps include:

- Degradation models that can be incorporated into techno-economic analysis
- Software tools and algorithms for capacity/expansion planning with high penetrations of inverter-based generation and energy storage
- Software tools and algorithms for optimal energy storage sizing and placement
- Optimal dispatch algorithms with extremely high penetrations of variable renewable generation (including curtailment)

3.7. Safety of Battery Energy Storage Systems (Joshua Lamb, Org. 2546)

3.7.1. Safety of Battery Energy Storage Systems – Background

High energy electrochemical storage systems are currently seen as the primary driver for enabling vehicle electrification as well as integrating new renewable energy technologies for energy distribution. However, in many areas, our understanding of the safety of these technologies, particularly when considering large battery systems, is limited. Sandia has dedicated facilities that are able to perform long-term reliability assessment and abusive testing on electrochemical energy storage devices from single cell batteries to modules up to 10s of kWh in size. This is complemented by substantial capability in performance and thermal modeling.

3.7.2. Safety of Battery Energy Storage Systems – Sandia Capabilities

Sandia has specific capabilities dedicated to better understanding the safety and reliability of electrochemical energy storage systems with a focus on high energy density batteries for electric vehicles and stationary applications. Facilities include the Battery Abuse Test Laboratory (BATLab), a DOE core facility for battery safety testing capable of performing destructive testing on cells and modules of up to 500 Wh, the burn site test facility for performing similar tests on battery systems of up to 25 kWh and the Energy Storage Analysis and Reliability Labs are equipped to conduct performance and lifetime testing on high energy cells, modules and packs.

Test facilities include:

- Battery Abuse Test Laboratory – Capable of destructive testing of batteries up to 500 Wh
- Burn site test facility – Capable of destructive testing of batteries up to 25 kWh
- Energy Storage Analysis and Reliability Labs– Performance and reliability testing of high energy battery systems
- Battery calorimetry testing – 4 Standard size and 2 enhanced volume accelerating rate calorimeters for studying the energetics of battery failure
- Destructive physical analysis – Physical disassembly of cells before and after abuse testing
- Materials characterization facilities
- Battery prototyping facilities
- Computed tomography (CT) scanning – 3d imaging of batteries before and after abuse testing

Sandia has played a pivotal role in understanding the safety of batteries, particularly for the development of lithium-ion batteries for vehicular and stationary applications. Sandia has also been able to employ its significant experience in combustion modeling to better understand the spread of battery failure and fires. Figure 15 shows details of various battery safety activities, and Table 9 provides a detailed summary of the capabilities devoted to battery safety and reliability testing.

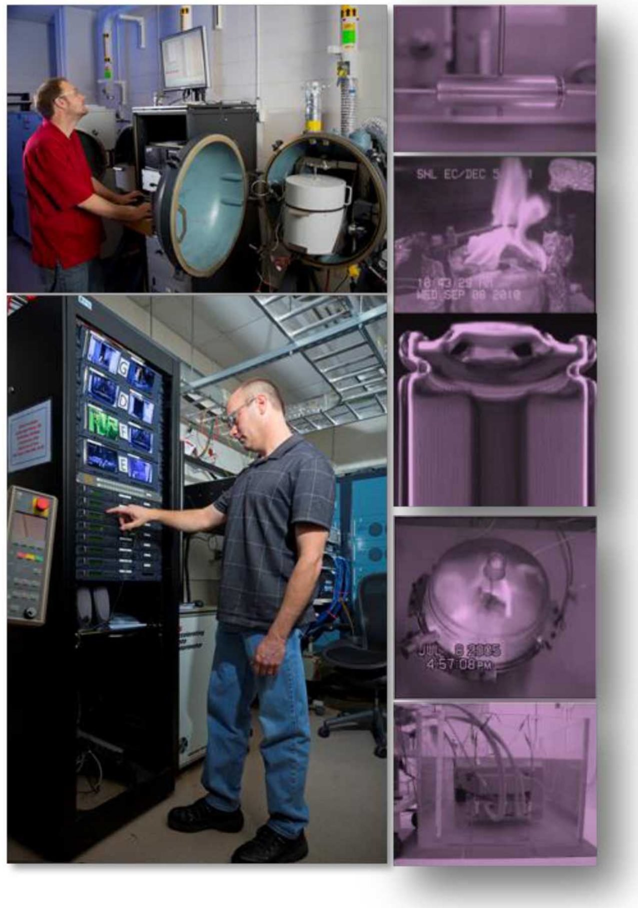
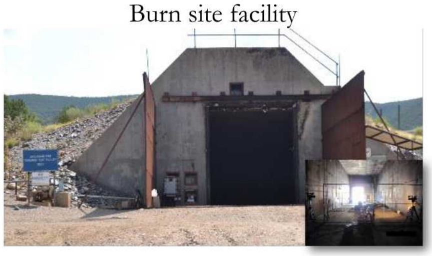


Figure 15. Battery abuse testing at Sandia.

Table 9. Summary of battery safety and reliability test capabilities.

Facility	Description
Battery Abuse Test Laboratory	The BATLab includes 6 reinforced test bays that are capable of withstanding abusive battery failures of high energy density batteries of up to 500 Wh in total stored energy. This includes a stand-alone exhaust ventilation system and closed circuit monitoring to ensure continuous monitoring of tests. General testing includes: • Overcharge/overvoltage • Overdischarge and voltage reversal • Over temperature testing • External short circuit with a minimum of 1 mOhm short resistance • Mechanical crush, nail penetration testing and dynamic impact (drop tower) This testing is accomplished with an array of data acquisition capabilities which include: • Voltage and temperature monitoring of >100 independent 0-10V voltage channels and thermocouple channels • High speed channels up to 1kHz data collection rates • Four 1000 V data channels

Facility	Description
	• Battery cyclers include up to 100V and 80 A, or up to 20V and 800 A. • Power supplies up to 600V • Hydraulic mechanical test equipment capable of up to 100 klb_f • Video monitoring • IR video monitoring
Burn site facility 	Batteries greater than 500 Wh stored energy, and up to 25 kWh stored energy are tested at the burn site facility. Testing and data acquisition capabilities from the BATLab have either been replicated or can be readily relocated to this facility. This also provides space for limited testing of large battery systems running beyond intended capabilities.
Energy Storage Analysis and Reliability Labs 	The Sandia Energy Storage Analysis and Reliability Labs are focused on providing the most accurate state of health (SOH) metrics for energy storage devices by bridging the gap between battery cell level studies and assessment of grid-scale units. This is accomplished by studying the fundamental processes that degrade batteries ranging from coin cells to kWh modules. The above objectives are enabled by a suite of commercial battery testers with hundreds of channels at voltages up to 72V and currents up to 1000A. Much of this testing is carried out with commercial components, however, collaborations with other battery facilities at Sandia enable the fabrication and testing of custom-made modules. Numerous thermal chambers (-72 °C to 95 °C) enable testing at controlled environmental conditions and impedance spectroscopy equipment enables the correlation of battery state of health to changes in battery electrical character. Full power electronics prototyping capabilities also allow batteries to be cycled under voltage and current profiles consistent with fielded systems.
Thermal runaway and battery propagation modeling	Computational and analytical modeling of runaway thermal heating and design mitigations.
Battery Calorimetry Testing	Accelerating Rate Calorimetry testing is used to quantify the thermal runaway behaviors of batteries. This includes four “standard” size calorimeters capable of tests of single cells of up to 3 Ah in capacity. Larger cells can be tested in the large format extended volume calorimeters. This allows more careful measurements of the onset temperatures of thermal runaway, peak heating rates, and total energy generated during thermal runaway. The standard calorimeters are pressure-tight, allowing for measurement of the total gas production during thermal runaway.
Destructive Physical Analysis	A dedicated glovebox is available for destructive physical analysis of cells both before and after testing. This can be used to observe the aftermath of a thermal runaway event, the effects of long-term aging on battery materials, and to aid in postmortem analysis of unexpected failure. Aged and abused electrode materials can also be harvested for further study in conjunction with materials analysis capabilities at Sandia.

Facility	Description
Battery Gas Analysis	Tools are available for studying the quantity and composition of vent gasses produced during abusive battery failures. FTIR and Mass spectrometry tools are available for in-operando testing of vent gasses prior to and during thermal runaway of batteries. More careful ex-situ analyses can be performed as well by collecting gas samples for external testing. Measuring the quantity of gas produced in large batteries is typically performed by initiating battery failure in either a 5 gal or 40 gal pressure vessel available for this testing.
Battery prototyping laboratories	Sandia maintains dry rooms containing battery prototyping facilities to build 18650 and pouch format cells. This enables controlled studies of new materials to determine their potential impact on battery safety. New materials and devices designed to improve battery safety can also be compared with a control cell to provide a careful evaluation of any potential improvements.
Materials Characterization	Sandia has developed world-class analytical facilities that include SEM, TEM, Auger, XPS, TOF-SIMS, FIB, XRD, and IR Spectroscopy. This allows for materials characterization to better understand the underlying mechanisms of thermal runaway and battery failure.
Computed Tomography (CT) scanning	Microfocus CT equipment is available for performing non-destructive imaging of batteries prior to and after abuse testing. This capability has proven particularly useful for evaluating the level of damage done during crush and nail penetration testing, as well as observing the aftermath of thermal runaway events inside the batteries tested.

3.7.3. Safety of Battery Energy Storage Systems – Gaps, Challenges, and Needs

Electrochemical energy storage devices, particularly lithium-ion batteries, present specific safety challenges. First among these is that a battery cannot simply be shut off. Truly deenergizing a system typically isn't possible. Managing the residual stored energy provides a specific challenge to the first and second response of a battery failure. As hundreds or thousands of cells can be used to create the full system, it is not uncommon to have a significant number of cells with an unknown state. These can reignite a battery fire and present a hazard during recovery efforts. During recovery, significant effort is often required to diagnose and discharge stored energy from a damaged system. A single cell failure can present a larger hazard if it is able to cascade to other cells in the system as well.

Lithium-ion makes up nearly all of the commercialized high energy systems and presents specific challenges. The active materials are typically not stable outside of normal operating conditions and must be regularly monitored to prevent a thermal runaway scenario. Many typical cathode materials have high rate exothermic decomposition reactions that lead to thermal runaway and battery fire events. The electrolyte used presents specific risks as well. The electrolyte is typically made up of low flashpoint organic solvents that readily degrade to flammable gasses such as H_2, CO, and CH_4. This can lead to a fuel-air conflagration if they are able to fill a confined space.

Historically battery safety testing has focused on single cells, but an approach more focused on the concerns of large battery systems and their failure modes is needed. This will require the development of test techniques to understand issues like cascading battery failure and ignition of the gasses produced during battery failure. There are also currently gaps in the understanding of battery failure as batteries age, particularly considering that the operating conditions that batteries will see in their lifetime can vary wildly from system to system. On-going research is focusing on these areas to ultimately drive a better understanding of both how battery systems might fail and improve the means to both prevent and respond to catastrophic battery failure. There is increasing analysis of how power electronics can be used to redistribute energy in order to reduce the risk of failure propagation in a system.

To date, most of the battery reliability and safety research at Sandia has focused on Li-ion batteries as they are the dominant technology for electrochemical grid energy storage. However, there are many promising aqueous battery technologies on the path to commercial adoption. Though aqueous batteries are considered lower risk, they can still undergo problematic degradation processes such as gas evolution. A modular device facility is needed to enable evaluation of different chemistries and components for redox flow batteries up to the stack level.

3.8. Testing, Demonstrations, and Model Validation (Ben Schenkman and Dan Borneo, Org. 8811)

3.8.1. Testing, Demonstrations, and Model Validation – Background

The Department of Energy Office of Electricity's (DOE-OE) mission is to work closely with private and public partners to ensure the nation's most critical energy infrastructures are secure and able to recover rapidly from disruptions. One area where Sandia supports this mission is its Electrical Energy Storage (EES) program. The program is made up of six thrust areas. One thrust area is the Industry Acceptance (IA) sub-program. IA collaborates with private and public partners to test and demonstrate Energy Storage Systems (ESS) with the goal to ensure EES systems are safe, reliable and cost effective. Sandia provides services to the industry through the multiple stages of developing and implementing and testing an ESS.

3.8.2. Testing, Demonstrations, and Model Validation – Sandia Capabilities

Sandia strives to help Energy Storage (ES) meet these challenges of improving the grid by collaborating with developers, academia, utilities, energy storage providers, and others to understand and improve ESS. Sandia's expertise allows us to:

- Provide initial analysis and modeling of the grid to determine the appropriate applications for the ESS, the need for distributed energy resources (DER), and the financial benefits of energy storage for the given markets
- Model ESS to determine size MW/MWh for optimum cost benefit
- Support the development of Requests for information (RFI) and Requests for Proposals (RFP)
- Review proposals and vet technologies
- Work with Partners to develop conceptual electrical designs and installation plans for Energy storage installations and other distributed energy resources in microgrids and power distribution systems
- Work with the project team to vet energy resources and operational control methods
- Review data collection plans

- Review contract documents to ensure requirement compliance
- Review safety features and annunciation/control means
- Vet commissioning plans and testing protocols for both factory tests and field installations
- Provide technical support during construction and commissioning
- Conduct operational performance data review and analysis
- Provide operational analysis and develop optimization algorithms

Within Sandia, two labs exist that provide R&D for ESSs being deployed. The Energy Storage Controls and Analytics Lab (ESCAL) provides R&D for residential and light commercial ESSs, and the Energy Storage Test Pad (ESTP) evaluates utility scale ESSs up to 1MW. ESCAL evaluates emerging technologies including their battery management systems (BMS) and energy management systems (EMS) before they are deployed in the field. This evaluation ensures the performance, reliability and safety of the system. The ESCAL has the capability to evaluate an ESS up to 30kVA, in a single phase (120V_{LN}) or three phase (208V_{LL}) configuration demonstrating various electrical grid conditions. The lab has an OPAL-RT which is a real-time simulator that replicates, through dynamic modeling, a specific electrical condition that an ESS may encounter when installed. OPAL-RT allows for a full utility electrical grid or a single building to be dynamically modeled, and the point of interconnection (POI) or point of common coupling (PCC) of the ESS to be evaluated. This lab uses a 37kVA regenerative power amplifier as power-hardware-in-the-loop controlled by the OPAL-RT, providing real electrical parameters, such as voltage and current, to an ESS under evaluation. High speed and precision data are collected from the ESS through a data acquisition system developed by A&D providing feedback to the OPAL-RT system. As part of the cost effectiveness evaluation, the ESSs are characterized to develop accurate models to be used within economic analysis software such as Quest and determine the limitations of the ESSs operating within certain applications or a combination of them.

ESTP was developed in 2010 to evaluate the validity and performance of utility scale ESSs. This lab consists of a concrete pad able to hold a 60' tractor trailer or iso-containers containing batteries or other energy storage mediums (Figure 16). Alongside this pad are various electrical panels rated at 480$V_{LL}$with multiple size breakers to connect ESSs from 10kW up to 1MW. These electrical panels are connected to a switchgear lineup that has a connection to the Sandia electrical distribution grid through a 480V_{LL}/12470V_{LL} step up transformer. This connection enables the ESS to be evaluated as a grid tied asset. A remote-controlled main breaker within the switchgear allows the ESTP to be isolated from the Sandia electrical grid. With the main breaker in the open position, the ESS can be assessed in an isolated or off-grid application. In addition, the ESS' transition from grid tied to island operation mode can be evaluated. Connected in parallel to the ESS within the switchgear is a 250kVA electrical feeder to the Distributed Energy Technology Laboratory (DETL). This allows for a microgrid connection with various loads and sources to be connected, including PV and generators. A 1MW/1MVAR (resistive and inductive) programmable load bank with 5kW/5kVAR steps is also connected to the switchgear. This load bank can replicate a load demand profile such as the load on a utility feeder or large industry complex that the ESS must respond to. Other generation sources that exist at the ESTP are three 60kW tactical quiet generators and a 250kW/1MWh UniEnergy Technologies (UET) vanadium redox flow battery. These sources can be used to replicate a forward operating base or small village electrical system incorporating an ESS. All the devices connected to the switchgear are monitored using Square D Powerlogic CM4000T power quality meters. These meters allow for high resolution of data capturing for power quality parameters such as harmonics. Controlling the utility scale ESS is done through the same A&D control and data acquisition system used in the ESCAL.

Figure 16. Energy Storage Test Pad (ESTP) at Sandia with a 1 MWh flow battery being tested.

The labs are physically separated by 7 miles and are connected through fiber lines as part of an internal Sandia network known as XNET. XNET connects multiple labs throughout Sandia into a single fiber network allowing the capability for one lab to communicate to other labs. Through this network, the ESTP can be controlled through the ESCAL which the latency in communication and their impact to the overall performance of the ESS can be evaluated. In both labs, innovative algorithms for a BMS or EMS can be implemented through the OPAL-RT software and provided to the ESS under evaluation. Both labs can be run together in a single test to evaluate two separate grids with various size ESSs. This setup allows the capability to evaluate networked microgrids consisting of ESS and other various sources.

3.8.3. Testing, Demonstrations, and Model Validation – Gaps, Challenges and Needs

ESSs are being installed at a rapid rate and standards for safety, control and interconnection are straining to keep up with the advancements. Forward thinking testing methods, using real-time simulators and facilities developed to incorporate a multitude of chemistries, are needed to provide input for these standards. Safety testing has typically been at the cell and module level of an ESS. Full system safety tests that include fire and explosion testing need to be conducted. Performance and operational data from ESSs are considered proprietary by many vendors, which makes it hard to collect, therefore making it hard to disseminate and understand the gaps in ESS technologies. This challenge needs to be overcome to allow all ESS vendors to learn and develop safer and more reliable systems for the end users. Economic analysis by the national labs and third-party consultants also require this data to have accurate models that provide a result with high level of confidence.

4. SANDIA DIVISION 8000 ENERGY STORAGE OPPORTUNITIES – 2020 TO 2030

The proposed energy storage capabilities roadmap for Division 8000 consists of near-term (1 – 2 years), mid-term (3 -5 years), and long-term (6 – 10 years) objectives (see Figure 17). These high-level objectives are guided by the key energy-storage gaps and challenges identified in this report that face Sandia and the nation as summarized in Section 4.2.

4.1. Timeline

As shown in Figure 17, the near-term objectives are to position Sandia and Division 8000 as a key player and leader in DOE's ESGC initiative. We have already led lab and regional workshops in 2020 and have contributed to the ESGC Roadmap. Additional efforts are currently underway to identify and coordinate capabilities in hybrid energy systems for DOE, which includes aspects of the ESGC and energy storage. Sandia is also planning to host a virtual long-duration ("Big Storage") energy storage workshop among national labs, industry, academia, utilities, and other stakeholders in the September – December 2020 timeframe. Finally, through development of this report and roadmap, investigators across Divisions 1000, 2000, and 8000 have initiated discussions to coordinate ideas and proposals for energy storage R&D.

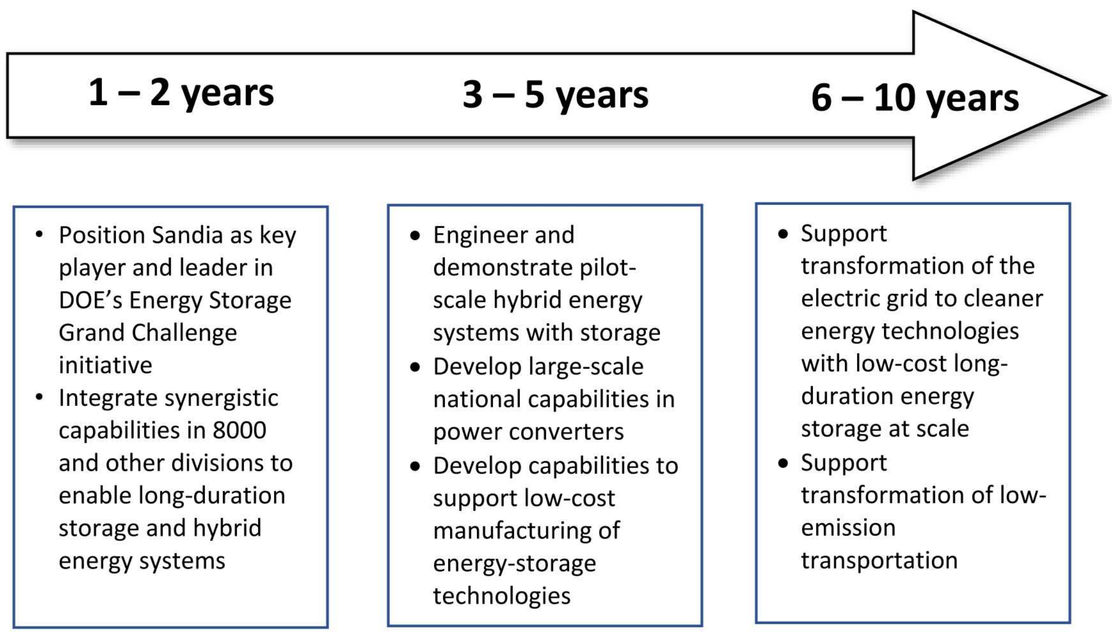


Figure 17. Summary of proposed Division 8000 Energy Storage Capabilities Roadmap.

The mid-term objectives focus on applying past and on-going R&D to develop demonstrations at pilot scales (~10 – 1000 kWh) for hybrid energy systems and large-scale power converters. Center 8800 has unique expertise, laboratories, and equipment that can position Sandia at the forefront of power conversion technologies, from advanced power electronics to next-generation power cycles (e.g., supercritical CO_2 Brayton cycles). Sandia also has capabilities in 1000 and 8000 to assist with the development of low-cost manufacturing of energy-storage technologies. Funding opportunities in LDRD and DOE FOAs or lab calls can support these objectives.

Finally, the longer-term goal is to support the transformation of the electric grid to cleaner energy technologies with low-cost long duration energy storage. Sandia has an opportunity to provide technical leadership in supporting New Mexico's Energy Transition Act to deliver carbon-free energy to New Mexico by 2045. If intermittent renewables will be the dominant source of electricity and energy, energy storage will play a critical role. Development and demonstration of large-capacity, long-duration energy storage technologies through next-generation storage technologies such as flow batteries, thermal/thermochemical storage, subsurface energy storage, and hydrogen storage is a significant opportunity for Sandia that will have enormous impacts for New Mexico, the nation, and DOE's mission for secure, resilient, sustainable energy.

Sandia's LDRD program should be leveraged to perform critical research activities that complement these objectives. Energy storage funding opportunities are also anticipated in upcoming DOE calls as part of the ESGC program and individual DOE offices. Sandia should utilize the collective research, resources, and capabilities identified in this report to respond to these calls.

4.2. Key Energy Storage Gaps and Challenges Facing Sandia and the Nation

- **Sandia Gaps and Challenges**
    - Coordinated research efforts across battery research teams to increase engagement and support for OE, JCESR, and LDRD programs
    - Equipment, methods, and capabilities to accelerate materials discovery for battery, thermal, and thermochemical storage technologies and power conversion technologies
    - Expertise and use of machine learning to optimize chemistries and formulations for storage materials (battery, thermal, thermochemical, hydrogen storage media and containment materials)
    - Techniques for low-cost, high-yield fabrication and manufacturing of materials, devices, and components for storage and power conversion
    - Development of facilities and engineered systems that demonstrate scale-up of lab-scale devices and materials with expected performance and reliability
    - Multiscale modeling that can be applied to scale-up of microstructure features and processes to engineered systems; developing appropriate constitutive relations for continuum-based models
    - Development of degradation models that can be incorporated into technoeconomic analyses
    - Development and application of software and tools for life-cycle analyses of energy storage technologies and applications
    - Optimal dispatch algorithms for high penetrations of renewables
    - Evaluation of the reliability and safety of large-scale energy-storage systems, especially batteries; current methods focus on single cells
    - Sharing of information and data with industry and lab partners
- **National Gaps and Challenges**

- Development of large capacity, long-duration (> ~1 – 100 GWh) energy storage technologies
- Identification of energy-storage use-case requirements, metrics, and valuation so that appropriate, cost-effective technologies can be researched and developed
- Technoeconomic analyses including total life-cycle costs (e.g., manufacturing to end-of-life costs and disposition) of various energy-storage technologies for comparison to use-case requirements
- Safety and reliability standards for large-scale energy-storage systems
- Integrated energy storage for electrical grid and transportation sectors including fast charging stations, smart-grid controls to enable bi-directional storage using electric vehicles, and real-time accounting for billing and compensation (blockchain opportunities)
- Infrastructure to enable large-scale hydrogen storage and conveyance

5. SUMMARY

We believe that energy storage presents significant opportunities for Division 8000 and Sandia to leverage current capabilities and activities that will benefit DOE's mission and the national interest through a secure and resilient energy system. This report has presented an overview of Sandia's key energy-storage research capabilities, challenges and needs, and a proposed roadmap and timeline to support DOE's ESGC mission to become a global leader in energy storage technologies, manufacturing, and supply chain by 2030.

5.1. Key Capabilities

Battery Storage Technologies: Key capabilities in battery storage technologies include materials synthesis (1800), characterization and diagnostic capabilities (1512 and 1800), battery assembly and cell prototyping (1800), cell/system testing facilities (1800, 8800).

Power Electronics and Power Conversion Technologies: Sandia has a number of unique power electronics facilities that develop and analyze conversion systems, wide bandgap semiconductor materials and devices, and advanced capacitors (8811). In addition, advanced thermal-to-electric power conversion systems are being researched in 8823 and 8841.

Subsurface Storage Technologies: Sandia has expertise in subsurface site characterization, laboratory and in-situ field testing, complex coupled thermal-mechanical-hydrological modeling of geologic formations, and wellbore life-cycle analyses (8860).

Thermal/Thermochemical Energy Storage: Sandia runs the National Solar Thermal Test Facility (8823), which is the nation's only large-scale concentrating solar power tower test facility, including capabilities to study advanced thermal-storage technologies using molten salts and solid particles.

Hydrogen Storage Technologies: Center 8300 has a number of laboratory capabilities to analyze and develop hydrogen storage and fuel cell technologies, including the Hydrogen Effects on Materials Laboratory, Hydrogen Transport and Transport Laboratory, and Hydrogen-Surface Interactions Laboratory.

Data Analytics, Systems Optimization, and Controls: Key capabilities and software include QuEST, EGRET/Prescient, dynamic modeling of energy storage, and algorithms for wide-area control and optimal dispatch of energy storage (8811). Additional data analytics and machine learning capabilities exist in Center 1400.

Safety of Energy Storage Systems: Key facilities to test and evaluate energy storage safety include the Battery Abuse Test Laboratory, Burn site test facility, Battery calorimetry testing, destructive testing, and computed tomography scanning (2500).

Testing, Demonstrations, and Model Validation: Sandia has large-scale testing facilities to demonstrate energy storage systems, include the Energy Storage Controls and Analytics Lab and the Energy Storage Test Pad, which have focused on battery storage technologies (8811). The NSTTF can also be used for large-scale testing of thermal storage technologies.

5.2. Key Challenges and Needs

Key challenges, needs, and cross-cutting energy-storage opportunities include the following:

- **Sandia Gaps and Challenges**

- Coordinated research efforts across battery research teams to increase engagement and support for OE, JCESR, and LDRD programs
- Equipment, methods, and capabilities to accelerate materials discovery for battery, thermal, and thermochemical storage technologies and power conversion technologies
- Expertise and use of machine learning to optimize chemistries and formulations for storage materials (battery, thermal, thermochemical, hydrogen storage media and containment materials)
- Techniques for low-cost, high-yield fabrication and manufacturing of materials, devices, and components for storage and power conversion
- Development of facilities and engineered systems that demonstrate scale-up of lab-scale devices and materials with expected performance and reliability
- Multiscale modeling that can be applied to scale-up of microstructure features and processes to engineered systems; developing appropriate constitutive relations for continuum-based models
- Development of degradation models that can be incorporated into technoeconomic analyses
- Development and application of software and tools for life-cycle analyses of energy storage technologies and applications
- Optimal dispatch algorithms for high penetrations of renewables
- Evaluation of the reliability and safety of large-scale energy-storage systems, especially batteries; current methods focus on single cells
- Sharing of information and data with industry and lab partners

- **National Gaps and Challenges**
  - Development of large capacity, long-duration (> ~1 – 100 GWh) energy storage technologies
  - Identification of energy-storage use-case requirements, metrics, and valuation so that appropriate, cost-effective technologies can be researched and developed
  - Technoeconomic analyses including total life-cycle costs (e.g., manufacturing to end-of-life costs and disposition) of various energy-storage technologies for comparison to use-case requirements
  - Safety and reliability standards for large-scale energy-storage systems
  - Integrated energy storage for electrical grid and transportation sectors including fast charging stations, smart-grid controls to enable bi-directional storage using electric vehicles, and real-time accounting for billing and compensation (blockchain opportunities)
  - Infrastructure to enable large-scale hydrogen storage and conveyance

5.3. Preliminary Roadmap and Timeline

The timeline for proposed activities described in this report is 10 years, divided into near-term (1 – 2 years), mid-term (3 – 5 years), and long-term (6 – 10 years) objectives. Near-term activities include taking an active and leadership role within DOE's ESGC initiative and hybrid energy systems activities. Sandia can utilize cross-cutting skills across 8000, 1000, and 2000 to identify technologies and methods to enable long-duration energy storage. Mid-term activities include development of engineered systems and pilot-scale hybrid energy systems with storage and power conversion. Projects focused on low-cost assembly and manufacturing are also needed. The long-term objectives include supporting and implementing transformation of the electric grid to cleaner energy technologies with low-cost, long-duration energy storage. These objectives will also complement and support the transformation of low-emission transportation technologies.

REFERENCES

[1] Akhil, A.A., 2015, DOE/EPRI Electricity Storage Handbook in Collaboration with NRECA, Sandia National Laboratories, SAND2015-1002, Albuquerque, NM.

[2] Denholm, P., J. Nunemaker, P. Gagnon, and W. Cole, 2019, The Potential for Battery Energy Storage to Provide Peaking Capacity in the United States, National Renewable Energy Laboratory, NREL/TP-6A20-74184, Golden, CO. https://www.nrel.gov/docs/fy19osti/74184.pdf,

[3] Copp, D.A., T.A. Nguyen, R. Thomson, R.H. Byrne, and B.R. Chalamala, 2019, Optimal Sizing of Distributed Energy Resources for 100% Renewable Planning, *Applied Energy*, **In press**.

[4] Siegel, N.P., 2012, Thermal energy storage for solar power production, *Wiley Interdisciplinary Reviews-Energy and Environment*, **1**(2), p. 119-131.

[5] Forsberg, C., P. Sabharwall, and H.D. Gougar, 2019, Heat Storage Coupled to Generation IV Reactors for Variable Electricity from Baseload Reactors: Changing Markets, Technology, Nuclear-Renewables Integration and Synergisms with Solar Thermal Power Systems, Massachusetts Institute of Technology, Idaho National Laboratory, Exelon, MIT-ANO-TR-185, INL/EXT-19-54909, Cabridge, MA.

[6] Moller, K.T., T.R. Jensen, E. Akiba, and H.W. Li, 2017, Hydrogen - A sustainable energy carrier, *Progress in Natural Science-Materials International*, **27**(1), p. 34-40.

[7] S., W., 2011, Borehole and Formation Analyses to Support CAES Development in Reservoirs, Sandia National Laboratories, SAND2011-2145, Albuquerque, NM.

[8] Gardner, W.P., 2013, Preliminary Formation Analysis for Compressed Air Energy Storage in Depleted Natural Gas Reservoirs A Study for the DOE Energy Storage Systems Program, Sandia National Laboratories, SAND2013-4323, Albuquerque, NM.

[9] Grubelich, M.C., Bauer, S. J. Cooper, P. W., 2011, Potential hazards of compressed air energy storage in depleted natural gas reservoirs, Sandia National Laboratories, SAND2011-5930, Albuquerque, NM.

[10] Bauer, S.J., Webb, S. W., 2000, Summary Report on studies and Analyses supporting Underground Aspects of a CAES Facility at Norton, Sandia National Laboratories, SAND2000-3111, Albuquerque, NM.

[11] Bauer, S.J., Gaither, K.N., Webb, S. W., Nelson, C., 2012, Compressed Air Energy Storage in Hard Rock Feasibility Study, Sandia National Laboratories, SAND2012-0540, Albuquerque, NM.

[12] Hogan, R.G., Tillerson, J. R., Beasley, R. R., 1980, Strategic Petroleum Reserve (SPR) geological site characterization report, Bryan Mound salt dome, Sandia National Laboratories, SAND80-7111, Albuquerque, NM.

[13] Park, B.Y., 2019, Geotechnical Concerns of Bayou Choctaw Strategic Petroleum Reserve and Explanations, Sandia National Laboratories, SAND2018-13783, Albuquerque, NM.

[14] Freifeld, B., Oldenburg, C., Jordan, P., Lechua, L., Perfect, S., Morris, J., White, J., Bauer, S., Blankenship, D., Roberts, B., Bromhal, G., Glosser, D., Wyatt, D., Rose, K., 2016, Well Integrity for Natural Gas Storage in Depleted Reservoirs and Aquifers, Sandia National Laboratories, SAND2017-0599, Albuquerque, NM.

[15] Gomez, S., Steve R. Sobolik, S., Matteo, E., Taha, M., Stormont, J., 2017, Investigation of wellbore microannulus permeability under stress via experimental wellbore mock-up and finite element modeling, *Computers and Geotechnics*, **83**, p. 168-177.

[16] Genedy, M., Kandil, U., Matteo, E., Stormont, J., Taha, M., 2017, A new polymer nanocomposite repair material for restoring wellbore seal integrity, *J. of Greenhouse Gas Control*, **58**, p. 290-298.
[17] Bauer, S.B., P. , Pyatina, T. , Sugama, T., 2020, *Thermal expansion, fluid flow, and thermal shock of cement and a cement/steel interface at elevated pressure and temperature*, in *Stanford Geothermal Workshop*, Palo Alto, CA,
[18] Matteo, E.N., McMahon, K., Camphouse, R. C., Dewers, T. A., Fuller, T., Jove-Colon, C., and J. Mohagheghi, 2019, Monitoring and Repair of Cement- Geomaterial Interfaces in Borehole and Repository Scenarios, Sandia National Laboratories, SAND2019-1174, Albuquerque, NM.
[19] Heath, J.E., Bauer, S.J., Broome, S.T., Dewers, T.A., and Rodriguez, M.A., 2013, Petrologic and petrophysical evaluation of the Dallas Center Structure, Iowa, for compressed air energy storage in the Mount Simon Sandstone, Sandia National Laboratories, SAND2013–0027, Albuquerque, NM.
[20] Bauer, S.J., Holland, J.F., Stone, C.M., 2008, Two and Three Dimensional Finite Element Analyses of the Praxair H_2 Cavern, Sandia National Laboratories, SAND2008-4423, Albuquerque, NM.
[21] Lord, A.S., 2009, Overview of Geologic Storage of Natural Gas with an Emphasis on Assessing the Feasibility of Storing Hydrogen, Sandia National Laboratories, SAND2009-5878, Albuquerque, NM.
[22] Weber, P.D.R., B.L. and Rudeen, D.K., 2016, SANSMIC user manual, Sandia National Laboratories, SAND 2016-8350, Albuquerque, NM.
[23] Ballard, S., Ehgartner, B. L., Berndsen, J., Myers, R., and McHenry, J., 1997, The CAVEMAN Cavern Pressurization Model, Sandia National Laboratories, SAND97-2952, Albuquerque, NM.
[24] Ballard, S., Ehgartner, B. L., 2000, CaveMan version 3.0: A software system for SPR cavern pressure analysis, Sandia National Laboratories, SAND2000-1751, Albuquerque, NM.
[25] Park, B.Y., 2018, Geomechanical Simulation of Big Hill Strategic Petroleum Reserve - Model Calibration, Sandia National Laboratories, SAND2018-13783, Albuquerque, NM.
[26] Park, B.Y., 2016, Prediction of Wellbore Failure Using an Equivalent Wellbore through the Combined Moment of Inertia Calculation, Sandia National Laboratories, SAND2016-3610C, Albuquerque, NM.
[27] Munoz-Ramos, K., Brainard, J. R., McIntyre, A., Bauer, S. J., Akin L. A. Nicol, K., Hayden, H., 2012, Technical Assistance for Southwest Solar Technologies Inc. Final Report, Sandia National Laboratories, SAND2012-5912, Albuquerque, NM.
[28] Andraka, C.E., J.M. Christian, C.M. Ghanbari, D.D. Gill, C.K. Ho, W.J. Kolb, T.A. Moss, E.J. Smith, and J. Yellowhair, 2013, Sandia Capabilities for the Measurement, Characterization, and Analysis of Heliostats for CSP, Sandia National Laboratories, SAND2013-5492, Albuquerque, NM.
[29] Turchi, C.S., Z.W. Ma, T. Neises, and M. Wagner, 2012, Thermodynamic Study of Advanced Supercritical Carbon Dioxide Power Cycles for High Performance Concentrating Solar Power Systems, *Proceedings of the Asme 6th International Conference on Energy Sustainability - 2012, Pts a and B*, p. 375-383.
[30] Allendorf, M.D., Z. Hulvey, T. Gennett, A. Ahmed, T. Autrey, J. Camp, E.S. Cho, H. Furukawa, M. Haranczyk, M. Head-Gordon, S. Jeong, A. Karkamkar, D.J. Liu, J.R. Long, K.R. Meihaus, I.H. Nayyar, R. Nazarov, D.J. Siegel, V. Stavila, J.J. Urban, S.P. Veccham, and B.C. Wood, 2018, An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage, *Energy & Environmental Science*, **11**(10), p. 2784-2812.

[31] U.S. Department of Energy. *Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Office*. Available from: https://www.energy.gov/eere/fuelcells/hydrogen-storage.
[32] U.S. Department of Energy. *Onboard Hydrogen Storage for Light-Duty Fuel Cell Vehicles*. Available from: https://energy.gov/sites/prod/files/2017/05/f34/fcto_targets_onboard_hydro_storage_explanation.pdf.
[33] U.S. Department of Energy. *Onboard Type IV Compressed Hydrogen Storage System - Cost and Performance Status*. Available from: https://www.hydrogen.energy.gov/pdfs/19008_onboard_storage_cost_performance_status.pdf.
[34] U.S. Department of Energy. *Hydrogen Class 8 Long Haul Truck Targets*. Available from: https://www.hydrogen.energy.gov/pdfs/19006_hydrogen_class8_long_haul_truck_targets.pdf.
[35] White, J.L., A.A. Baker, M.A. Marcus, J.L. Snider, T.C. Wang, J.R.I. Lee, D.A.L. Kilcoyne, M.D. Allendorf, V. Stavila, and F. El Gabaly, 2020, The Inside-Outs of Metal Hydride Dehydrogenation: Imaging the Phase Evolution of the Li-N-H Hydrogen Storage System, *Advanced Materials Interfaces*, **7**(7).
[36] Schneemann, A., J.L. White, S. Kang, S. Jeong, L.W.F. Wan, E.S. Cho, T.W. Heo, D. Prendergast, J.J. Urban, B.C. Wood, M.D. Allendorf, and V. Stavila, 2018, Nanostructured Metal Hydrides for Hydrogen Storage, *Chemical Reviews*, **118**(22), p. 10775-10839.
[37] Sandia National Laboratories. *Hydrogen Storage*. Available from: https://energy.sandia.gov/programs/sustainable-transportation/hydrogen/storage/.
[38] Sandia National Laboratories. *Material & Components Compatibility*. Available from: https://energy.sandia.gov/programs/sustainable-transportation/hydrogen/materials-components-compatibility/.
[39] Liu, Y.S., L.E. Klebanoff, P. Wijeratne, D.F. Cowgill, V. Stavila, T.W. Heo, S. Kang, A.A. Baker, J.R.I. Lee, T.M. Mattox, K.G. Ray, J.D. Sugar, and B.C. Wood, 2019, Investigating possible kinetic limitations to MgB2 hydrogenation, *International Journal of Hydrogen Energy*, **44**(59), p. 31239-31256.
[40] Melaet, G., V. Stavila, L. Klebanoff, and G.A. Somorjai, 2018, The effect of aluminum and platinum additives on hydrogen adsorption on mesoporous silicates, *Physical Chemistry Chemical Physics*, **20**(17), p. 12075-12083.
[41] Ray, K.G., L.E. Klebanoff, J.R.I. Lee, V. Stavila, T.W. Heo, P. Shea, A.A. Baker, S. Kang, M. Bagge-Hansen, Y.S. Liu, J.L. White, and B.C. Wood, 2017, Elucidating the mechanism of MgB2 initial hydrogenation via a combined experimental-theoretical study, *Physical Chemistry Chemical Physics*, **19**(34), p. 22646-22658.
[42] White, J.L., A.J.E. Rowberg, L.W.F. Wan, S. Kang, T. Ogitsu, R.D. Kolasinski, J.A. Whaley, A.A. Baker, J.R.I. Lee, Y.S. Liu, L. Trotochaud, J.G. Guo, V. Stavila, D. Prendergast, H. Bluhm, M.D. Allendorf, B.C. Wood, and F. El Gabaly, 2019, Identifying the Role of Dynamic Surface Hydroxides in the Dehydrogenation of Ti-Doped NaAlH4, *Acs Applied Materials & Interfaces*, **11**(5), p. 4930-4941.
[43] Wood, B.C., V. Stavila, N. Poonyayant, T.W. Heo, K.G. Ray, L.E. Klebanoff, T.J. Udovic, J.R.I. Lee, N. Angboonpong, J.D. Sugar, and P. Pakawatpanurut, 2017, Nanointerface-Driven Reversible Hydrogen Storage in the Nanoconfined Li-N-H System, *Advanced Materials Interfaces*, **4**(3).
[44] Witman, M., S.L. Ling, D.M. Grant, G.S. Walker, S. Agarwal, V. Stavila, and M.D. Allendorf, 2020, Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data via Interpretable Machine Learning, *Journal of Physical Chemistry Letters*, **11**(1), p. 40-47.

[45] Eyer, J. and G. Corey, 2010, Energy Storage for the Electricity Grid: Benefits and Market Potential Assessment, Sandia National Laboratories, SAND2010-0815, Albuquerque, NM
[46] Vazquez, S., S.M. Lukic, E. Galvan, L.G. Franquelo, and J.M. Carrasco, 2010, Energy storage systems for transport and grid applications, *IEEE Transactions on Industrial Electronics*, **57**(12), p. 3881-3895.

DISTRIBUTION

Email—Internal

Name	Org.	Sandia Email Address
Technical Library	01977	sanddocs@sandia.gov

This page left blank

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.