Overview of the Advanced Battery Materials Research (BMR) Program and the Battery500 Consortium

Tien Q. Duong
Vehicle Technologies Office (VTO)
Energy Efficiency & Renewable Energy (EERE)
U.S. Department of Energy
Washington, DC 20585

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### Introduction

**Energy Storage R&D Interactions at DOE**

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<thead>
<tr>
<th>Fundamental Research</th>
<th>Transformational Research</th>
<th>Applied Research</th>
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<tr>
<td><strong>Office of Science</strong></td>
<td><strong>Advanced Research Projects Agency – Energy</strong></td>
<td><strong>Vehicle Technologies Office</strong></td>
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<tr>
<td>Fundamental research to understand, predict, and control the interactions of matter and energy at the electronic, atomic, and molecular levels</td>
<td>High-risk transformational research</td>
<td>Advanced Batteries for Automotive applications</td>
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<tr>
<td>- JCESR (energy storage hub)</td>
<td>- BEEST (high energy)</td>
<td>- Full system development &amp; testing</td>
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<td>- EFRC</td>
<td>- AMPED (battery sensors and controls)</td>
<td>- High-energy density &amp; high-power density cells</td>
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<tr>
<td>- Core scientific research</td>
<td>- RANGE (flow, solid state, multifunctional)</td>
<td>- Advanced battery materials research (BMR)</td>
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<td></td>
<td>- IONICS (solid state)</td>
<td>- Battery500</td>
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<td>- Extreme fast-charging</td>
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Fiscal Year 2017: $101M
Introduction (2)

DOE National Laboratory System

- Energy storage R&D currently pursued at 11 of the 17 DOE national laboratories
Advanced Battery Materials Research (BMR) Program

- Previously known as:
  - Exploratory Technology Research (ETR) (1980-2001)
    - Exclusively focused on batteries for automobile applications since 1992
  - Batteries for Advanced Transportation Technologies (BATT) (2002-2014)

- Charter: Perform cutting edge research in new materials and conduct comprehensive modeling and diagnostics analyses of materials and electrochemical cell behavior to address chemical, physical and mechanical instabilities

- 11 Topic areas, 63 research projects

  - Modeling (10), Diagnostics (9), Cell Analysis (4), Silicon Anodes (2), Intercalation Cathodes (8), Polymer/Liquid/Self-Healing Electrolytes (7), Solid State Electrolytes (4), Metallic Lithium (6), Sulfur Electrodes (9), Air Electrode/Electrolyte (3), and Sodium (1)
BMR: Current Participants

- BMR participants include 7 national labs, 20 universities, and 4 industry partners

<table>
<thead>
<tr>
<th>National Labs</th>
<th>Academia</th>
<th>Industry</th>
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<tbody>
<tr>
<td>Argonne National Laboratory</td>
<td>BYU</td>
<td>DAIKIN</td>
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<td>Brookhaven National Laboratory</td>
<td>Stanford University</td>
<td>GM</td>
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<td>Oak Ridge National Laboratory</td>
<td>Stony Brook University</td>
<td>Hydro Québec</td>
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<td>NREL</td>
<td>Rutgers</td>
<td>LIOX</td>
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<tr>
<td>Pacific Northwest National Laboratory</td>
<td>Texas A&amp;M University</td>
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Vehicle Technologies Office
Energy Storage R&D Program Structure

- The BMR program is one of the three key energy storage R&D programs in VTO

**Advanced Battery Materials Research (BMR Program)**
- SEM of Li$_2$FeSiO$_4$/C Nanospheres
- High capacity cathodes
- Alloys, and lithium metal anodes
- High voltage electrolytes
- Solid State electrolytes

**Cell Materials Targets**
- Anode capacity > 1000mAh/g
- Cathode capacity > 300mAh/g
- High-voltage cathodes & 5V stable electrolytes
- Solid-polymer electrolytes with $>10^{-3}$ S/cm ionic conductivity

**High Energy & High Power Cell R&D (ABR Program)**
- Electrodes exhibiting high energy density and high rate capability
- Fabrication of high energy density cells
- Cell diagnostics
- Improved manufacturing processes

**Cell Targets**
- 350 Wh/kg
- 750 Wh/l
- 1,000 cycles
- 10+ calendar year life

**Full System Development & Testing (Developer Program)**
- Focus on cost reduction, life and performance improvement
- Robust battery cell and module development
- Testing and analysis
- Battery design tools
- Fast charge

**Battery Pack Targets**
- $125/kWh EV pack cost
- Fast charge (80% SOC in 15 minutes)
- $180, 12V start/stop pack cost
BMR Program in Context of VTO
Battery R&D

Technology Progression Example: Advanced Cathode Materials

- **Materials R&D**
  - Lithium-rich NMC
  - 1999–2015

- **Materials Scale Up and low Cost Processing**
  - BASF
  - 2007–2013

- **Cells & Electrochemistry Development**
  - Lithium-ion Polymer, Mixed Mn/NMC–Carbon, USABC
  - 2005–2014

Commercialization
Research Emphasis on Li-ion Batteries (1)

Cathodes

- **Barrier**: Electrode capacity – still a limiting factor

Approaches

- **Develop Ni-rich cathodes** that exhibit stable operation at high voltage with long cycle life
- **Optimize the composition** of structurally-integrated Li-rich ‘layered-layered’ and ‘layered-layered-spinel’ to mitigate voltage fade during cycling
- **Discover new materials**: gain fundamental understanding of the role of O₂ in Li-excess cathodes

![Voltage Profiles for Li-rich, Layered Cathode](chart1)

High-Capacity Li-Excess Oxides

![Graph showing voltage profiles for Li-rich, layered cathode](chart2)

Source: BATT projects
Research Emphasis on Li-ion Batteries (2)

Silicon Anode

- **Barrier:** Continuous formation of the SEI during cycling consumes lithium and solvent

Approaches

- **New architectures:** Design of novel morphologies and configurations; e.g. nanotubes, nanowires, core-shell and nanocomposite structures

- **Development of functional coatings:** metals, Li\(^+\) and e\(^-\) conducting ceramics including high strength and elastomeric polymer binders

(Note: most of the research projects in this area have been transferred to the ABR program.)
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Research Emphasis on Li-ion Batteries (3)

Electrolytes

- Current focus: Explore fluorinated carbonate and sulfone solvents

Approaches

- Understand reactivity at voltages above 4.3V
- Design new electrolytes and additives
- Maintain current focus on fluorinated carbonate, and sulfone solvents

Fluorinated Sulfone Molecules
(3D structure)

NMC532/Graphite Cells
(C/3 for 500 cycles, cut-off voltage 3.0-4.6 V)
Li-metal Based Batteries: Enabling A New Class of Electrodes

Potential Benefits
- Li metal anodes allow doubling of energy density. Enabling new class of high capacity cathodes, such as sulfur and other non-lithiated structures

Status
- Lithium reactivity and dendrite growth remain primary challenges

Approaches
- Additives/solvents to planarize deposition
- Polymers to compress protrusions
- Ceramics with high Li-ion conductivity
- Novel framework structures for lithium storage and cycling

Future Issues
- Enable use and operation of functional polymers at room temperature
- Generate interlayers to protect reaction of Li-metal with ceramics
- Processing of thin, brittle ceramic layers
- Maintain compression stability over Li diffusion lengths exceeding 10’s of microns
- Need for consistent testing protocols
Li-Sulfur Batteries: High Specific-Energy System

**Potential Benefits**
- Inexpensive, abundant material that promises high specific energy compared to Li-ion

**Status**
- Polysulfide “shuttle” and deposition of insoluble polysulfides remain challenges

**Approaches**
- Constraining the polysulfide within the cathode
- Development of separators with blocking ability
- Mechanistic understanding of speciation

**Future Issues**
- Operation of cathodes with high sulfur loading
- Understanding speciation in different electrolytes
- Operating under low electrolyte volumes (lean electrolyte)
- Co-locating the electrochemically oxidized and reduced products to ensure reversibility
- Ensure isolation of Li metal from the polysulfide species
Solid-State Batteries: A Path to Safer Li Metal-based Batteries

Potential Benefits
- Solid electrolytes provide a unique path to lithium metal anodes while enabling safer operation

Status
- Current focus on Li conducting lanthanum zirconate ceramic structures (LLZO) and sulfide based glasses

Approaches
- All-polymer systems e.g. PEO
- All inorganic systems with ceramic integrated into porous cathodes

Future Issues
- Develop polymers with high room temperature Li-ion conductivity
- Ceramics with both high- and low-voltage stability
- Integrate ceramics into porous cathode structures with intimate contact
- Can we demonstrate an all solid-state Li-ion battery with similar performance to liquid-based systems?
- Can Li-metal be stabilized to withstand abuse-tolerance?

Scalable and reproducible process to fabricate multilayer garnet structures
With surface treatment, Li metal wets garnet surface continuously inside porous support
Battery500 Consortium: Overview

### Timeline
- **Start date:** September 2016
- **End date:** September 2021
- **Percent complete:** 20%

### Barriers
- **Barriers to overcome**
  - Address the grand scientific and technological challenge:
    - Increase the energy density of advanced lithium (Li) metal batteries beyond the current state of Li-ion batteries

### Partners
- **Project lead:** Pacific Northwest National Laboratory
- **Partner Institutions:**
  - Binghamton University, Brookhaven National Laboratory, Idaho National Laboratory, SLAC, Stanford University, University of California San Diego, University of Texas at Austin, University of Washington
- **Other Partners:** Seedling project teams
Battery500 Consortium: Team

Battery500 Quarterly Review/Annual Meeting, SLAC, Jan 19, 2017
The Battery500 Consortium aims to triple the specific energy density (to 500 Wh/kg) relative to current battery technology with achievement of 1,000 charge/discharge cycles.

The consortium aims to overcome the existing fundamental scientific barriers and harvest the maximum capacity of electrode materials in two systems: Li metal-high Ni NMC and Li-S.

The consortium leverages the advances made in the research on electrode materials and battery chemistries supported by DOE.
Advanced Materials to meet Battery500 Goals

- Achieve dendrite-free Li deposition with more than 99.9% Coulombic efficiency.
- <100% excess Li (compared to cathode).
- Increase cathode capacity to over 220 mAh/g and achieve stability over 4.4 V.
- Increase stability window of electrolytes and achieve interfacial stability at both cathodes and anodes.
- Develop thick (>120 mm) and dense (<23% porosity) electrode architectures.
- Reduce inactive materials (electrolyte, current collectors, separator).
- Optimize materials properties at the cell level.
Battery500 Consortium: Keystone Projects

Harvest Maximum Capacity from Promising Battery Chemistries
High Ni NMC-Li: achieving >50% of theoretical capacity at cell level
Solid State Li-S: solving polysulfide dissolution and Li degradation problems

1. Materials/Interfaces:
   Mixed conductive coating
   Controlled surface reaction

2. Electrode Architecture
   Thick, conductive cathode
   3D Li composite structure

3. Cell Design/Integration
   Cell modeling
   1D or 2D Li⁺ conductor
   De-coupled SEI reactions

Diagnosis & prognosis, assessment and validation

Seedling projects: emerging concepts, alternative cathodes, 3D printed architectures, layer-by-layer fabrication of solid electrolytes, etc.

Technology exit strategies to improve Li ion batteries
- Li batteries
  - 500 Wh/kg
  - 1000 cycles
- New test beds or spin-off entities for technology scale-up in the US

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Summary & Conclusions

- VTO’s demonstrated track-record of success
  - NiMH batteries now used in commercial HEVs
  - Li-ion technologies being introduced in commercial PHEVs/EVs
  - American-based battery factories supplying batteries for several car companies

- Clear pathway to meet 2022 goals
  - 2022 cost goal: reduce production cost of an EV battery to $125/kWh
  - Major focus: Develop advanced Li-ion cells using higher voltage cathodes & intermetallic anodes
  - Expanded work: low-cost materials, electrode and cell manufacturing

- BMR technologies beyond 2022 and Battery500 Consortium
  - Continued focus on Li metal, sulfur electrodes and solid state electrolytes
  - Closely coordinated with the DOE Office of Basic Energy Sciences and other DOE offices
Energy Efficiency & Renewable Energy

THANK YOU!

For more information, contact:

Tien Q. Duong
Manager, Advanced Battery Materials Research (BMR) Program, and VTO
Battery500 Consortium
Battery R&D
Vehicle Technologies Office
Office of Energy Efficiency & Renewable Energy
U.S. Department of Energy

Tien.Duong@ee.doe.gov
(http://bmr.lbl.gov)