Overview and Progress of the Batteries for Advanced Transportation Technologies (BATT) Activity

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Project ID: **ES108**

Perform cutting-edge research on new materials and address fundamental chemical and mechanical instability issues.

Challenges

- Conduct research and development on the next-generation of battery anodes, cathodes, and electrolytes.
- Understand failure mechanisms to enable higher energy, longer lasting, and less expensive batteries.
- Conduct comprehensive modeling of cell and material behavior.

Battery R&D Budget

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Battery/Energy Storage R&D Funding ($, M)	
FY 2012* Enacted	$90
FY 2013 Full Year CR**	$88
FY 2014* (request)**	$170.5

*FY 2012 SBIR/STTR removed.
**FY 2013 full year CR inclusive of SBIR/STTR.
*** FY 2014 budget request inclusive of SBIR/STTR.

FY 2013 Energy Storage R&D Budget** ($88M)

Participants

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Argonne National Laboratory

ASU Arizona State University

Brookhaven National Laboratory

University of Cambridge

Binghamton University

Case Western Reserve University EST. 1826

MIT Massachusetts Institute of Technology

Stanford University

University of Pittsburgh

Berkeley Lab Lawrence Berkeley National Laboratory

Pacific Northwest National Laboratory

The University of Texas at Austin

Penn State Nittany Lions

Drexel University

Hydro Québec

GM

The University of California 1868 Let There Be Light

Texas A&M University

North Carolina State University

BYU

SwRI®

UC San Diego

NREL

Oak Ridge National Laboratory

The University of Rhode Island

Current BATT Portfolio

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High-Voltage Cathode
- Ni/Mn Spinel

High-Energy Anode
- Silicon

Novel electrodes, electrolytes, and separators

Novel additives

Novel electrode processing

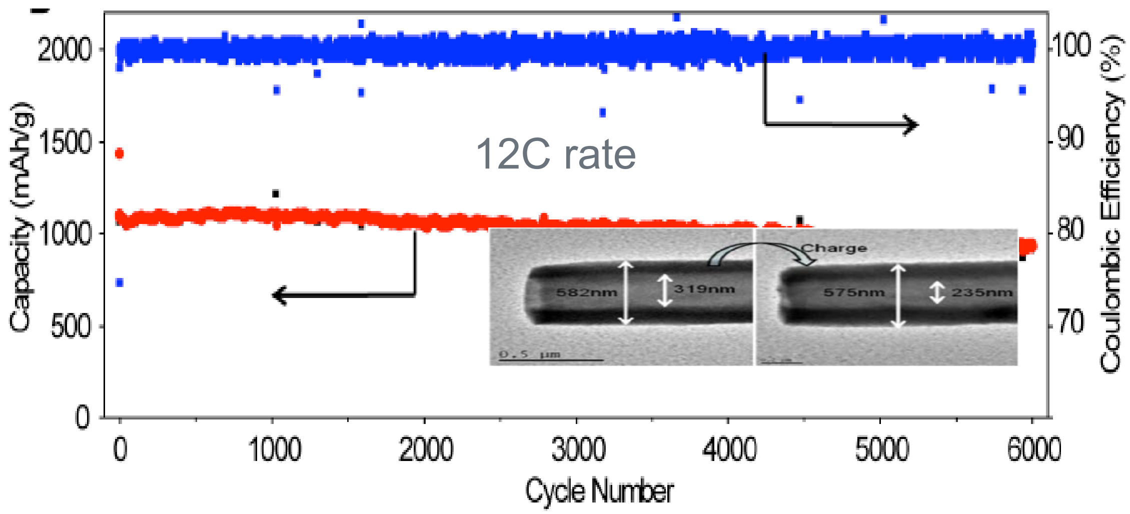
Beyond Li-ion
- Li-metal anode
- Li-S
- Li-air

Beyond Lithium
- Sodium?
- Magnesium?

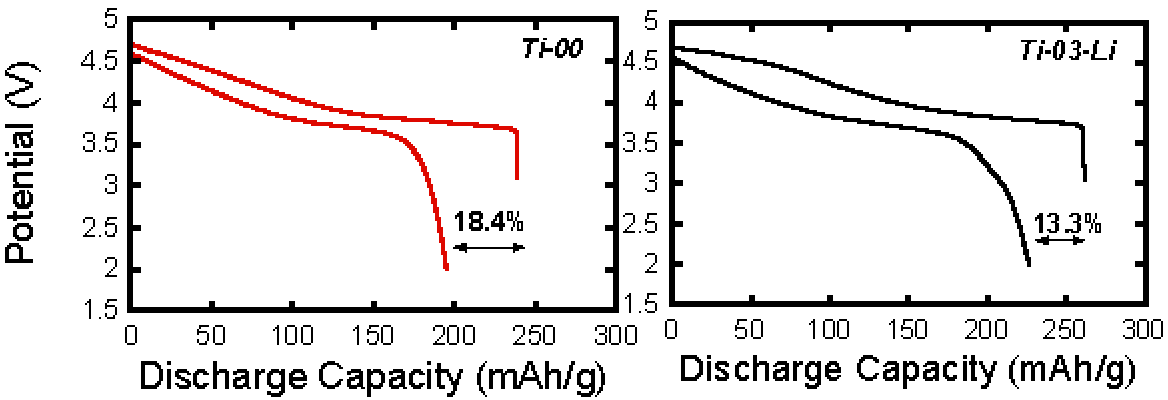
Specific System And Material Research → New Materials/ Processing Research → Beyond Li-ion Chemistry Research

1-3 years | 3-5 years | 5-10 years

Electrode Materials

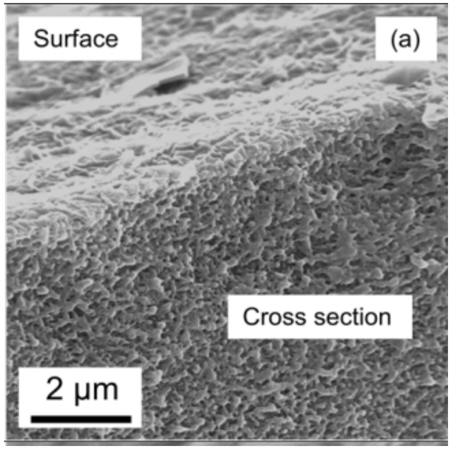


- Silicon nanotube electrodes show potential to eliminate cracking and exhibit excellent cycling capability (Cui, Stanford)



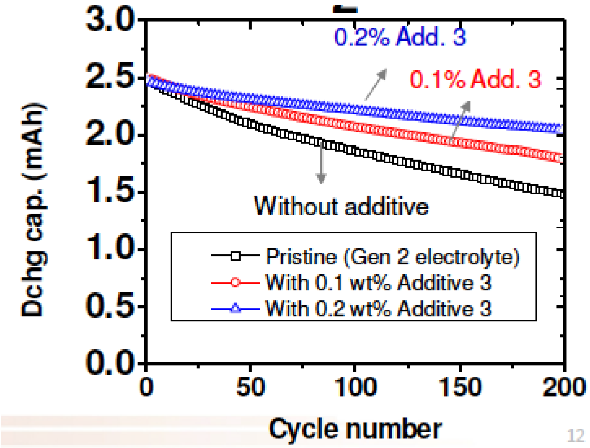
- Ti-doped NMC cathodes show promise with capacities of 225 mAh/g with improved cycling at higher voltages (Doeff, LBNL)

Electrolytes, Additives, Separators



- Self-assembled separators using a low-cost wet process show promise. Ionic conductivities in membrane comparable to Celgard. (Balsara, LBNL)

- 3-oxabicyclohexane-2,4-dione additive, predicted by modeling, shows promise in improving cyclability by forming a better SEI. (Amine/Curtiss, ANL)



Advanced Diagnostics, Modeling, and Assembly of Battery Materials and Electrodes

- 170 white papers received
- 54 full proposals requested
- 15 proposals awarded

Cell Development

Investigator	Institution	Project
Yet-Ming Chiang, Antoni Tomsia	MIT LBNL	*Design and Scalable Assembly of High Density Low Tortuosity Electrodes*
Gao Liu	LBNL	*Hierarchical Assembly of Inorganic/Organic Hybrid Si Negative Electrodes*
Karim Zaghib	Hydro-Québec	*Assembly of Battery Materials and Electrodes*

New Projects (2 of 3)

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Modeling

Investigator	Institution	Project
Gerbrand Ceder	MIT	*First Principles Calculations of Existing and Novel Electrode Materials*
Kristin Persson	LBNL	*Understanding and Predicting Novel Electrode Materials from First-Principles*
Dean Wheeler, Brian Mazzeo	Brigham Young University	*Predicting Microstructure and Performance for Optimal Cell Fabrication*
Yue Qi, Xingcheng Xiao, Huajian Gao, Brian Sheldon, Yang-Tse Cheng	General Motors Brown University University of Kentucky	*A Combined Experimental and Modeling Approach for the Design of High Current Efficiency Si Electrodes*
Perla Balbuena, Jorge Seminario, Kevin Leung, Susan Rempe	Texas A&M University Sandia National Laboratories	*First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anode*

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Diagnostics

Investigator	Institution	Project
Clare Grey	University of Cambridge	*NMR and Pulse Field Gradient Studies of SEI and Electrode Structure*
Robert Kostecki	LBNL	*In-situ Characterization of Interfaces and Interphases in Electrical Energy Storage Systems with Far- and Near-Field Multiprobe Techniques*
Guoying Chen	LBNL	*Optimization of High-energy Electrode Materials*
Nitash Balsara, David Prendergast Jordi Cabana	University of California, Berkeley LBNL	*Active Binders for High-energy Density Cathode*
Xiao-Qing Yang, Kyung-Wan Nam	BNL	*Advanced in-situ Diagnostic Techniques for Battery Materials*
Gabor Somorjai, Phillip Ross	University of California, Berkeley LBNL	*Analysis of Film Formation Chemistry on Silicon Anodes by Advanced in-situ and operando Vibrational Spectroscopy*
Shirley Meng	UC San Diego	*Optimization of Ion Transport in High-energy Composite Cathodes*

Collaboration and Coordination

- **Basic Energy Sciences**
  - Energy Frontier Research Centers
  - Joint Center for Energy Storage Research
    - Multivalent Intercalation
    - High-throughput calculations and datamining of advanced electrolytes
- **ARPA-E**
  - Lithium/Air and Lithium/Sulfur chemistries

FY 2014 Plans

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- Solicit new proposals for Novel Electrolytes and Additives
  - Primary focus on single ion conducting membranes
  - Request for concepts papers announced: January 2014

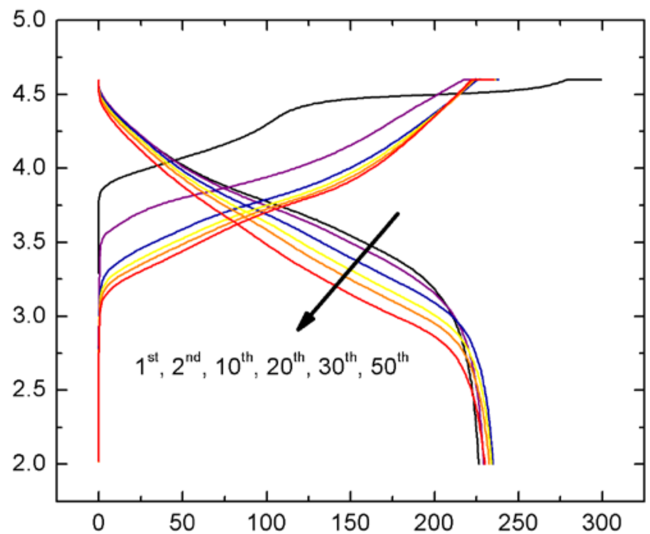
Mid-Term R&D: Advanced Lithium-ion (1)

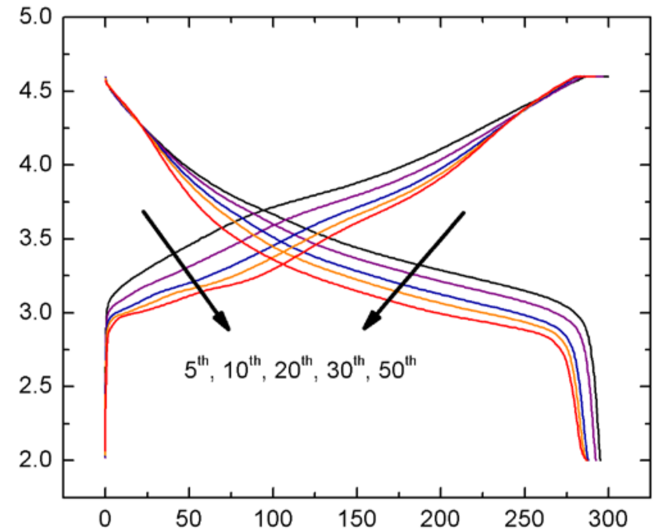
Issues

- Advanced anode materials (Sn and Si) have large storage capacities (>1,000 mAh/g), but they undergo a significant volume change
  - Have large irreversible capacity loss.
  - Consume electrolyte due to a continuing forming of the SEI layer.
- Stability of Li-rich, layered-cathode ($xLi_2MnO_3 \bullet (1-x)LiMO_2$), spinels and phosphates at high operating voltages remains problematic
  - Current electrolytes are not stable above 4.3V.
  - Metal dissolution resulting in poor performance and short cycle life.
  - Structure of the material changes during cycling causing voltage fade.

Mid-Term R&D: Advanced Lithium-ion (2)

Voltage profiles of $Li/0.5Li_2MnO_3 \bullet 0.5LiNi_{0.44}Co_{0.25}Mn_{0.31}O_2$ cells cycled at C/15 rate





Approach

- Current research includes new synthesis routes, development of novel electrolytes and additives, and applying coatings on particles and electrodes.

Resolving these issues would make feasible an advanced lithium-ion cell with specific energies of 300–350 Wh/kg

Long-Term R&D: Beyond Li-ion (1)

Beyond Li-ion chemistries would likely require use of metallic lithium

Li-Metal Anode Issues

- Dendrite formation resulting in loss of lithium and possible safety hazard
- Solvent reduction also resulting in loss of lithium and electrolyte

Approach

- Decouple lithium metal from cathode chemistry
  - Block co-polymers
  - Single-ion conducting ceramics
  - Multiple ceramic/polymer stabilization layers

Protection of lithium metal surface from chemical interactions is critically important for beyond Li-ion batteries

Long-Term R&D: Beyond Li-ion (2)

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Not many options for high-capacity cathodes – still the limiting electrode

- Non-intercalation, low-cost, and high-capacity cathode materials
  - LiV_3O_8: 280 mAh/g, V_2O_5: 441 mAh/g, and others (TBD)
  - Sulfur: 1,675 mAh/g
  - O_2: still have reservations on air electrode

Sulfur Cathode Issues

- Dissolution of lithium polysulfides leading to high self-discharge
- Insoluble sulfur species such as Li_2S_2 and Li_2S could passivate the electrodes
- Practical specific energy is 2 times better, but energy density is comparable to Li-ion battery

Approach

- Confining the polysulfides in core shell or yolk shell nanostructures
- New solvents, additives and dual electrolyte systems