Overview of the Batteries for Advanced Transportation Technologies (BATT) Program

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OVT Merit Review

This presentation does not contain any proprietary or confidential information

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BATT Program Mission

- The BATT program performs **fundamental research** in support of the DOE/EERE FreedomCAR and Vehicle Technologies Program to develop batteries for vehicular applications (EV, HEV, and Plug-in hybrid)
- Presently, the focus is on lithium-based systems (Li-ion and Li-metal)
- Consists of 23 PIs from various universities, national labs, and one company
- Program lead: Prof. John Newman, UC-Berkeley

Critical Challenges*

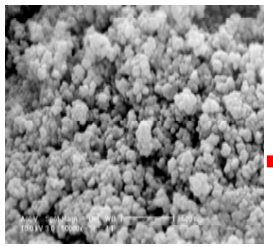
- Cost
- Life
- Abuse tolerance
- Performance (low-temperature operation, energy, and power)

Choice of application decides the critical problems to be solved:

- EV: Need double the energy density of presently available Li batteries
- HEV: low-T operation, cost, and abuse tolerance
- Plug-in hybrid: life (especially calendar life), cost (related to energy)

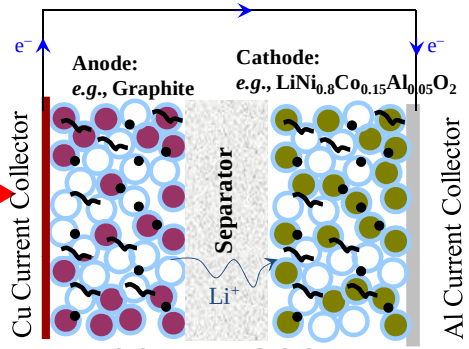
* See DOE Multi-year Plan

Material Synthesis, Diagnostics, and Modeling Across Length Scales



10 nm-10 μm

Length Scales



100 μm-300μm

Structural Diagnostics

Electrochemical Diagnostics

Electrode Diagnostics

Electrochemical Analysis

Material Synthesis/ Modifications

New/Improved Material

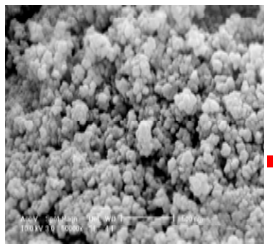
Electrode/Battery Fabrication

Improved Chemistry

Structural Modeling

Electrode Modeling

Material Synthesis, Diagnostics, and Modeling Across Length Scales



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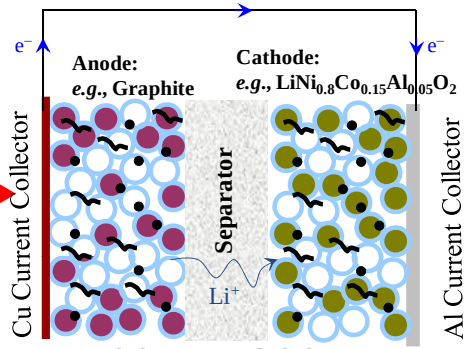


100 μm-300μm

Grey, Kostecki, Shao-Horn, Yang/Yoon

Kerr, Kostecki, West

Thackeray, Kumta, Whittingham, Doeff, Goodenough, Balsara, Manthiram, Richardson, Desmarteau/Creager

New/Improved Material

Battaglia, Dudney, Zaghib

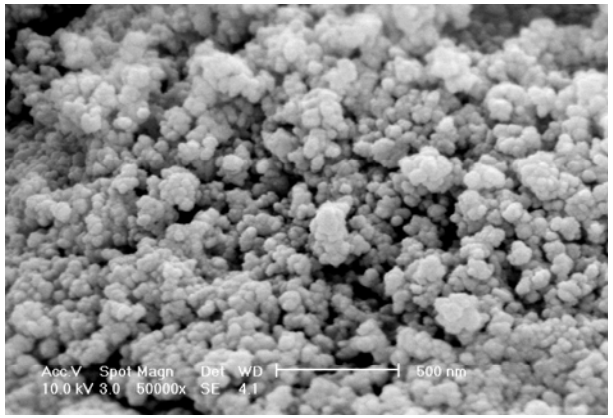
Improved Chemistry

Ceder, Smith/ Borodin

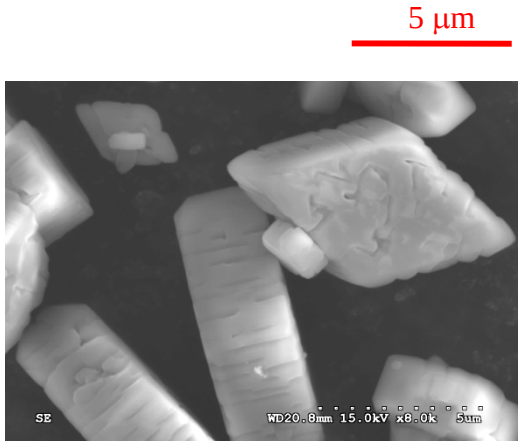
Newman, Sastry, Wheeler, Srinivasan

Material Synthesis Across Length Scales

Low conductivity of lithium iron phosphate necessitates the synthesis of nanoparticles to allow material to operate at high rates.



G. Ceder (MIT)

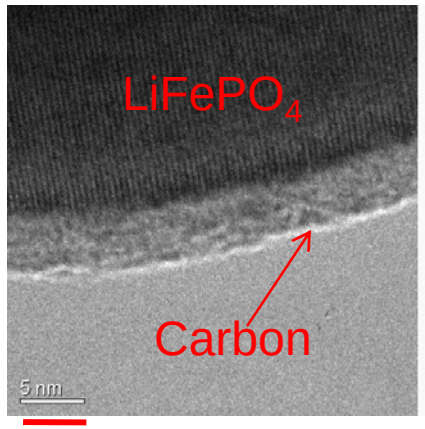


T. Richardson and G. Chen (LBNL)

Micron-sized lithium iron phosphate particles provide an elegant means of studying mechanism of lithium intercalation and may hold the key to high-energy batteries

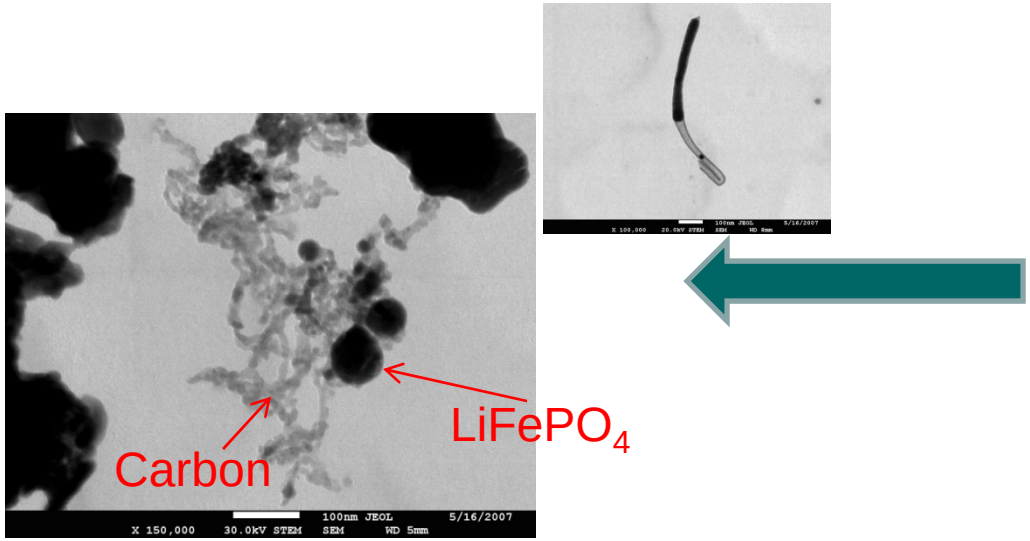
Material Modifications on the Nanoscale

Low conductivity of lithium iron phosphate necessitates the use of a thin carbon coating on the particle to enhance conduction on the particle-scale.



5 nm

H. Gabrisch (U. New Orleans),M. M. Doeff (LBNL)

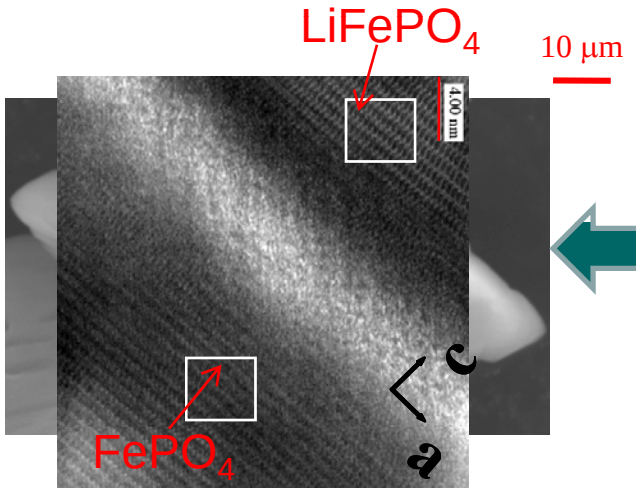


100 nm

M. M. Doeff (LBNL)

In situ growth of carbon nanotubes while synthesizing lithium iron phosphate allows good particle-to-particle conduction.

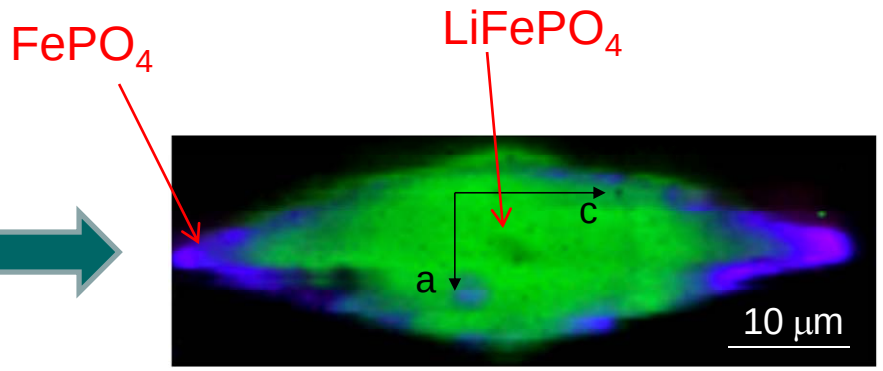
Spectroscopic Diagnostics Across Length Scales



T. Richardson and G. Chen (LBNL)

Detailed TEM analysis allows for identification of evolution of phases in the nanoscale during battery cycling.

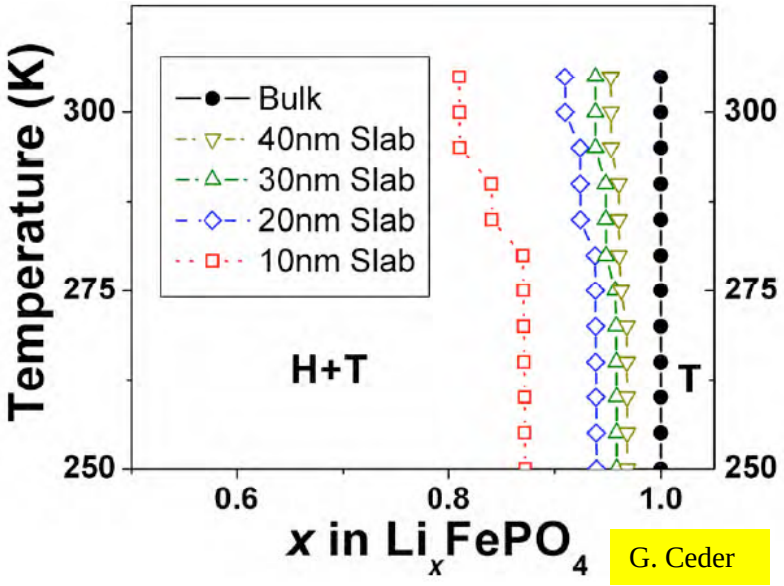
Raman maps on the particle-scale show the anisotropy of the process.



R. Kostecki, T. Richardson, G. Chen (LBNL)

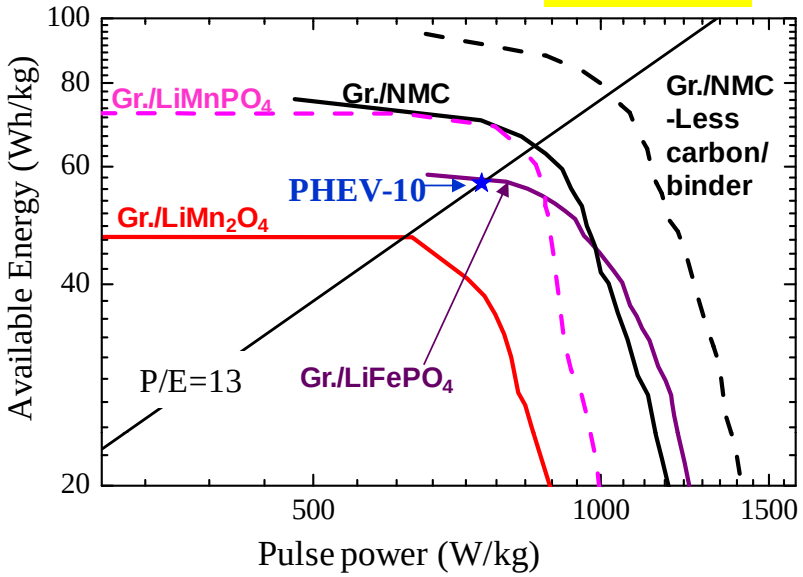
Computer Simulations Across Length Scales

Monte Carlo simulations allows prediction of solubility limits of Li in $LiFePO_4$



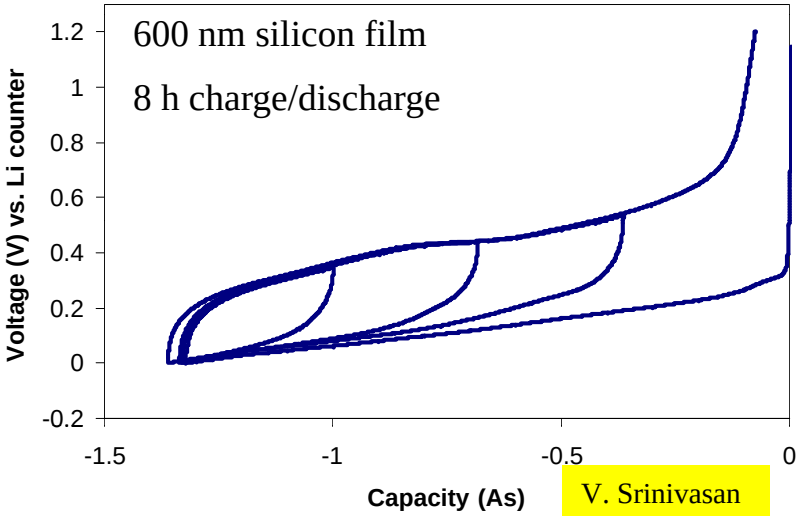
G. Ceder

V. Srinivasan



Continuum modeling allows correlation of material properties to performance. Simulations allow for accessing ability of materials to satisfy vehicular applications

Electrochemical Analysis

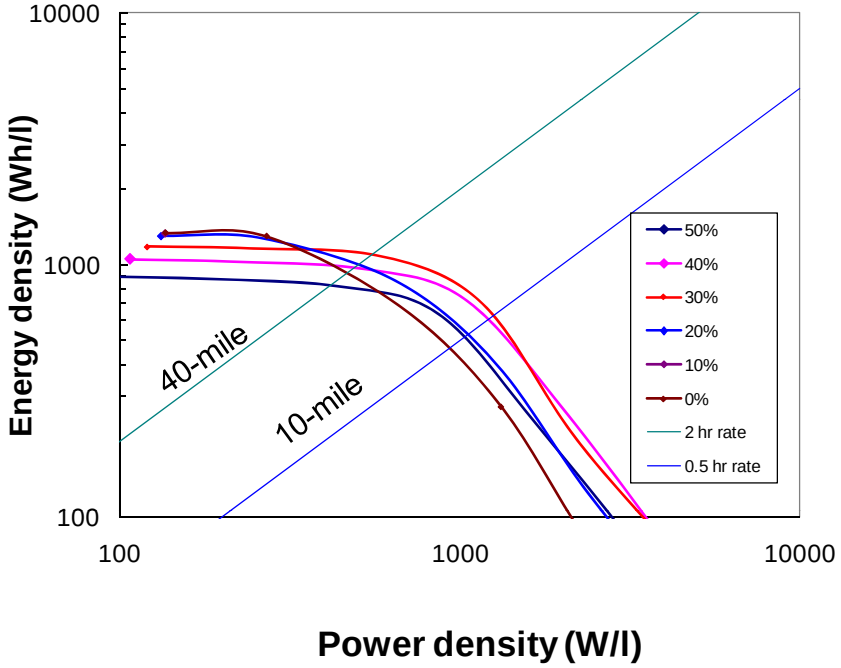


V. Srinivasan

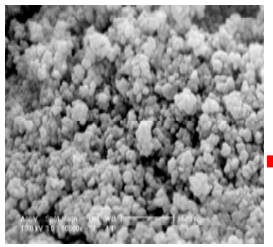
Thin-film electrodes allow detailed investigation of the active material without complexity of the porous network

V. Battaglia and G. Liu

Experiments on test cells allow for identification of ideal formulation to meet requirements.



Material Synthesis, Diagnostics, and Modeling Across Length Scales



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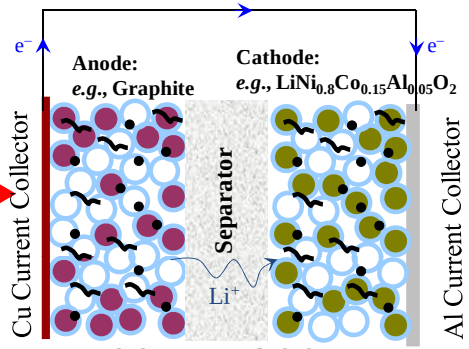

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Reviewer Comments from June 2006 BATT Review

1. Investigate higher-energy anodes
2. Continue SEI work
3. Consider developing high-voltage electrolyte, additives *etc*

Search for next-generation materials

4. Fund projects each year that are more high risk
5. Add ultracapacitor research to the program
6. Consider high-rate and low-temperature carbon research
7. Transfer Al-corrosion work to the ATD project
8. Reduce work on ionic liquids and Solid Polymer Electrolytes
9. Control water level in all experiments

BATT Discussion Meeting in June 2007

- Talks on DOE perspective, BES workshop conclusions, and ATD Program.

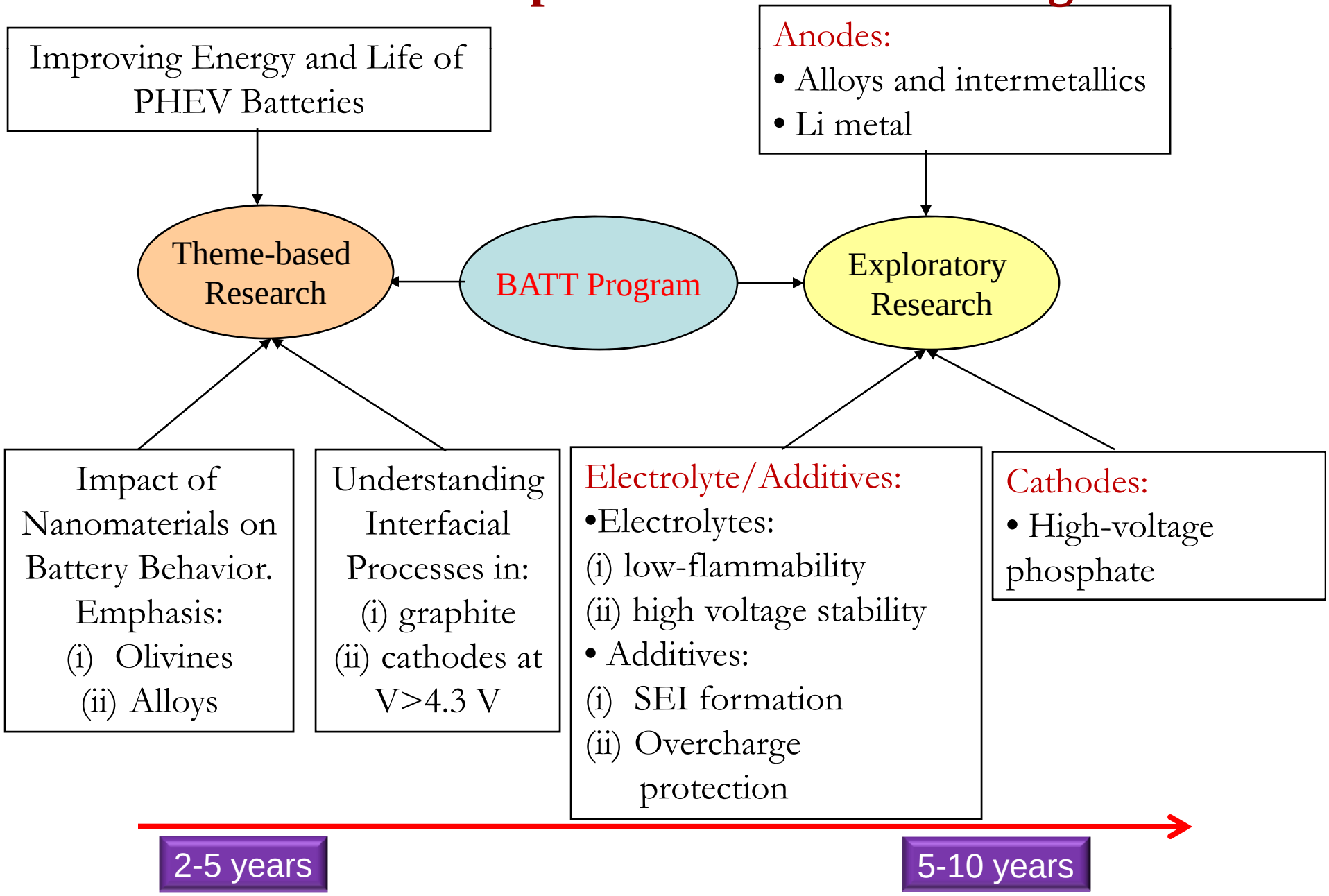
- PIs split into six topic areas (Cathodes, Anodes, Electrolytes/Interfaces, Diagnostics, Modeling, and Cell Analysis) or *panels*

- *Panel leads* made a brief presentation summarizing present focus and ideas for future areas of research
  - Mike Thackeray, ANL
  - Stan Whittingham, SUNY
  - Phil Ross, LBNL
  - Clare Grey, SUNY
  - Gerd Ceder, MIT
  - Vince Battaglia, LBNL

- Presentations were used to initiate discussion

Main Focus: Decreasing cost and abuse tolerance and increasing life of **high-energy PHEV batteries**

Present Emphasis of the BATT Program



Request for Proposals (RFP)

- BATT has issued a RFP in the area of "**Synthesis and Characterization of Novel Electrolytes and Additives for Use in High-energy Lithium-ion Batteries**"

- Emphasis on:
  - Electrolytes: High voltage, low cost, high flammability, high stability
  - Additives: Stable film (SEI) forming, overcharge protection

  - 43 responses were received to a request for a white-paper (from various Universities, National Labs, and companies)

  - All proposals were reviewed by a panel of experts on Li-ion batteries

  - 21 whitepapers were approved by the panel have been asked to submit a final proposal

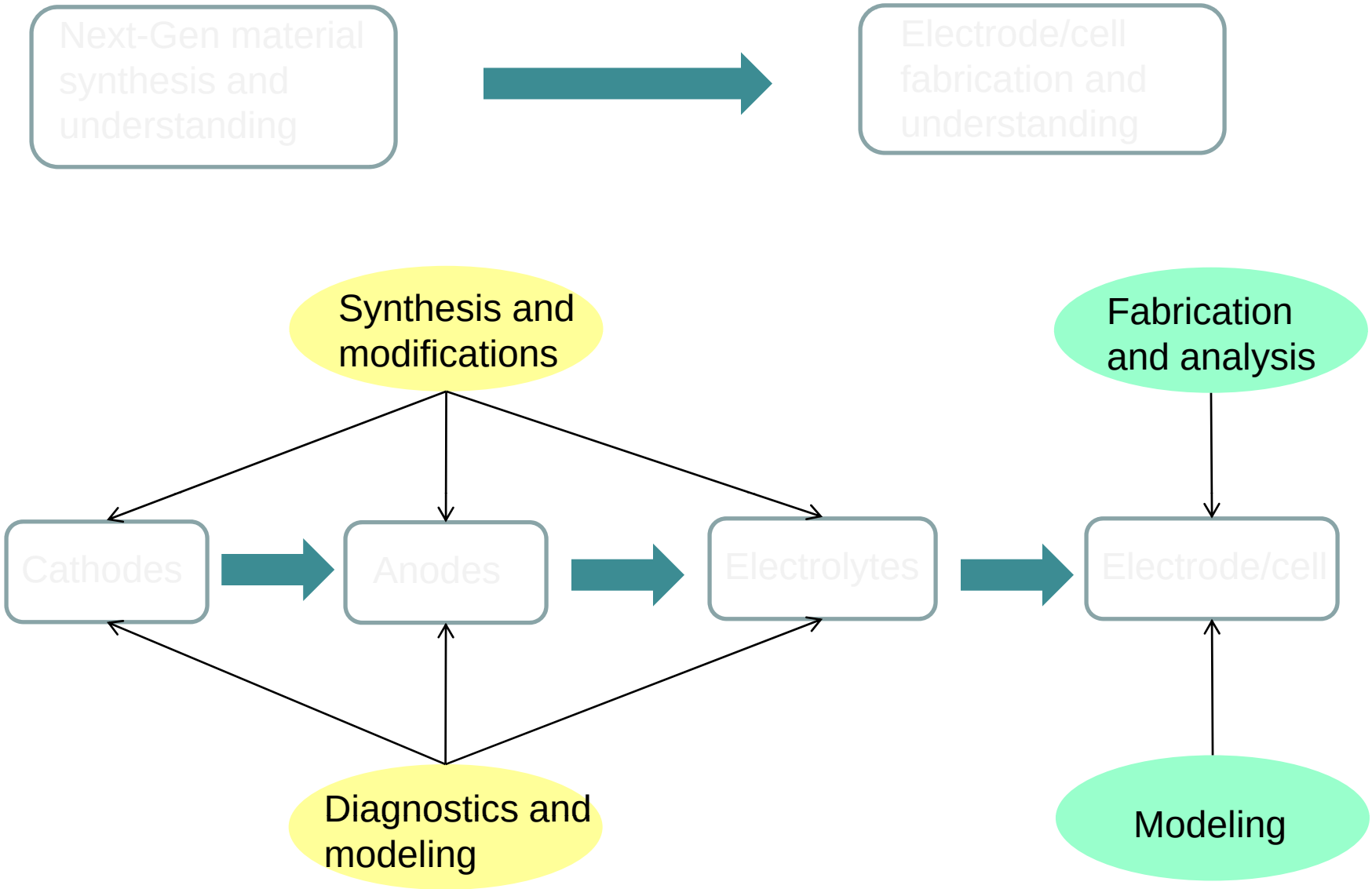
  - All 21 will be subjected to an independent review process

  - We anticipate 2-3 new subcontracts to be placed in Summer 2008

BATT is always looking for new ideas that advance the mission of DOE/BATT.

See http://berc.lbl.gov/BATT/BATT.html for details on how to submit a proposal.

Review Agenda



Acknowledgements

- BATT Program participants
  - Especially Frank McLarnon, Vince Battaglia, and John Newman

- DOE Office of FreedomCAR and Vehicle Technologies

For additional information see http://berc.lbl.gov/BATT/BATT.html

BATT Program Projects

- **Cell Analysis**
  - Cell Fabrication and Materials Characterization (Battaglia)
  - Cathodes, Alloy Anodes, Diagnostics (Richardson)
  - Lithium-Ion Batteries with Low-Cost Materials (Zaghib)
  - Design and Fabrication of High-performance Lithium-ion Electrodes for PHEVs (Wheeler/Harb)
  - Investigation of Metallic Lithium Anode and Graphite Current Collector for Advanced Batteries (Dudney)

- **Anodes**
  - Intermetallic anode development and characterization (Thackeray)
  - Preparation and characterization of alloy anodes (Whittingham)
  - Studies on the Li-metal interface (West)
  - *High Capacity Reversible Nanoscale Heterostructures: Novel Anodes for Lithium-ion Batteries (Kumta)-Project initiated Dec. 2007*

- **Electrolytes**
  - Development of Polymer Electrolytes for Advanced Lithium Batteries (Balsara)
  - Electrolyte design, characterization, and interfacial processes (Kerr)
  - Lithiated Fluorosulfonimide Ionomers as Multifunctional Binders/Electrolytes in Battery Cathodes (DesMarteau/Creager)
  - Molecular Modeling of Electrode/Electrolyte Interfaces (Smith/Borodin)

- **Cathodes**
  - Composite layered manganese oxide cathodes (Thackeray)
  - Stabilized layered manganese oxides, low-temperature synthesis (Whittingham)
  - Synthesis and Characterization of Cathode Materials for Rechargeable Lithium and Lithium-ion Batteries (Doeff)
  - High-capacity $LiNi_{0.5}Mn_{0.5}O_2$ cathodes (Goodenough)
  - High-Performance Cathode Materials (Manthiram)

- **Diagnostics**
  - Interfacial Processes: Diagnostics, Nanomaterials (Kostecki)
  - XRD, XAS, *etc*. of Battery Materials(Yang)
  - First-principles calculations and NMR of cathode materials (Ceder/Grey)
  - Studies and Design of Chemically and Structurally Stable Surfaces of Lithium Storage Materials (Shao-Horn)

- **Modeling**
  - Thermodynamics, rate processes, failure mechanisms, analysis (Newman)
  - Understanding the Behavior of Advanced Li-ion Chemistries Using Mathematical Modeling (Srinivasan)
  - Mesoscale Simulations of Active Materials for High-Power Batteries: Interrogation of Failure Mechanisms during Cycling (Sastry)