Breakout Report on Energy Storage

Identification of Grand Challenges
Energy Storage Breakout

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20 year Grand Challenge

“To know all reactions occurring in a battery system and their rates, so that you can identify importance of, and select or exclude, each one.”

Cross-cutting themes:
• Discovery of new materials
• Identification of new storage mechanisms
Grand Challenge 1: Five Years to Five Volts

If materials scientists could elucidate bulk and interfacial reaction mechanisms for all plausible electrolytes (including solids) at 5V, then stable new high energy density battery systems become possible.
Grand Challenge 2: Accelerated Identification of Long-Term Failure Modes

If materials scientists could identify and quantify low-rate degradation mechanisms, then materials process engineers could:

• Reduce testing time (from current time of several years)
• Speed up implementation of new materials
• Speed up development of new battery systems, e.g.:
  – Li-ion (e.g., high Mn systems)
  – Beyond Li-ion (e.g., metal-sulfur)
Grand Challenge 3: Accelerating Synthesis

If researchers and developers could predict the outcome of synthesis processes, the design and testing of new materials, and their incorporation into battery systems, would be greatly accelerated.

- Emphasis on data collection and computation for the inorganic chemist
- The inorganic chemist does not have the same vast data base that the organic chemist has today
- “Pourbaix-like diagram + kinetics”
Other ideas

Other:
- Enabling metal anodes
- Linking physical properties with electrochemical properties
- Linking to downstream manufacturing processes - “Virtual manufacturing environment”
- Creating a multiscale virtual battery
- The ultimate non-flammable electrolyte
- Theory and modeling of additives and trace impurities
- Extending the stability window of aqueous systems – the 3V aqueous battery