



Basic Research Needs for Electrical Energy Storage

Report of the Basic Energy
Sciences Workshop on
Electrical Energy Storage
April 2-4, 2007



CONTENTS

	Page
Figures.....	v
Abbreviations, Acronyms, and Initialisms.....	vii
Executive Summary of the DOE Basic Energy Sciences Workshop	ix
Introduction.....	1
Basic Research Needs for Electrical Energy Storage	7
Chemical Energy Storage	9
Capacitive Energy Storage.....	16
Priority Research Directions	23
Novel Designs and Strategies for Chemical Energy Storage.....	25
Solid-Electrolyte Interfaces and Interphases in Chemical Energy Storage	31
Capacitive Energy Storage Materials by Design	37
Electrolyte Interactions in Capacitive Energy Storage	41
Multifunctional Materials for Pseudocapacitors and Hybrid Devices.....	47
Rational Materials Design Through Theory and Modeling.....	53
Cross-cutting Science for Electrical Energy Storage.....	65
Advances in Characterization	67
Nanostructured Materials.....	69
Innovation in Electrolytes	72
Theory, Modeling, and Simulation	74
Conclusion	77
Appendix A: Technology and Applied R&D Needs for Electrical Energy Storage.....	A-1
Appendix B: Probing Electrical Energy Storage Chemistry and Physics Over Broad Time and Length Scales	B-1
Appendix C: Workshop on Basic Research Needs Electrical Energy Storage.....	C-1

FIGURES

Figure	Page
1. A battery system involves interactions among various states of matter.....	12
2. The large concentrations of dislocations in commercial LiCoO ₂ , as revealed by transmission electron microscopy raise fundamental questions with direct bearing on battery function.....	12
3. Power density as a function of energy density for various energy storage devices	18
4. Schematic illustration of the cation arrangement in a layered, composite $x\text{Li}_2\text{MnO}_3 \bullet (1-x)\text{LiMn}_{0.5}\text{Ni}_{0.5}\text{O}_2$ electrode structure in which LiMn ₆ units, characteristic of the Li ₂ MnO ₃ component (and disordered LiMn ₅ Ni units), are embedded as stabilizers in the residual LiMn _{0.5} Ni _{0.5} O ₂ component.....	26
5. Three-dimensional nanostructure demonstrating the intergrowth of the anode, cathode, and electrolyte	28
6. Operation principle, interphase formation, intra-electrode and intra-cell interfaces in lithium-ion cells	31
7. A proposed model of the electrode near a complex SEI	32
8. SEI stability and growth during continuous lithium uptake and removal for different anodes: graphite, lithium storage metals, and metallic lithium.....	33
9. LiODFOB: a hybrid electrolyte salt material formed from LiBF ₄ and LiBOB	34
10. Schematic of an activated carbon-based EDLC illustrating the heterogeneity of particle size, pore size, and pore structure of the electrode that ultimately leads to performance limitations	37
11. Cagey structures	39
12. Ions in the ionic liquids (a) <i>N</i> -methyl- <i>N</i> -propylpyrrolidinium bis(trifluoromethanesulfonyl)-imide (PYR ₁₃ TFSI) and (b) 1-ethyl-3-methylimidazolium tetrafluoroborate (EMIBF ₄)	43
13. Schematic of how ion solvation may change in pores of different sizes during electric double layer charging (electrode material, black; solvent, blue; cation, orange, anion, red)	43

14. Calculated and scaled Raman spectra for (a) $\text{Et}_4\text{N}^+ D_{2d}$ (solid line) and S_4 (dotted line), (b) TFSI ⁻ transoid C_2 (solid line) and cisoid C_1 (dotted line) compared with (c) experimental Raman spectrum of Et ₄ NTFSI recorded at 296 K	44
15. Transmission electron micrograph of nanocomposite of RuO ₂ and the conducting polymer, PAPPA.....	51
16. (Left) Sketch of a single electrode layer of a carbon-based EC illustrating the hierarchical pore structure with macropores between carbon agglomerates and micro-to-nanopores inside agglomerates.....	55
17. Breakdown of circuit models in nonlinear charging dynamics	59
18. (Left) Atomic configuration of propylene carbonate in a carbon slit obtained by reverse Monte Carlo simulations from X-ray diffraction measurements on Maxsorb92-16 porous carbon with a surface area of 2440 m ² /g and a pore size of 1 nm	60
19. Molecular-dynamics simulations of an EC consisting of a periodic carbon nanotube forest in a common organic electrolyte (1 M TEA + BF ₄ ⁻ in propylene carbonate)	61
B.1. Normalized Mn(a), Ni(b), and Co(c) K-edges XANES of $\text{Li}_{1-x}\text{Co}_{1/3}\text{Ni}_{1/3}\text{Mn}_{1/3}\text{O}_2$ as a function of the amount of lithium in the lattice.....	B-6
B.2. Imaging lithium in a block copolymer electrolyte	B-7
B.3. A multifunctional imaging nanoprobe.....	B-8