LIB – Optimization of the Electrodes, Collectors, and/or Separators in Li-ion Electrochemical Systems

Problem Statement

OBJECTIVE: To create novel approaches for the design and development of scalable hierarchical materials for improved electrodes, collectors and separators in Li-ion batteries with enhanced performance across a wide range of temperatures.

DESCRIPTION: The US Army needs long-lasting, gun-hardened batteries to address the new extended ranges required for the Army's number one modernization priority, Long Range Precision Fires. Lithium-ion batteries (LIBs) have been the dominant solution for the portable energy needs of myriad military and commercial applications.

The performance of LIBs in terms of high energy and power density is unparalleled. The development of alternative chemistries has not advanced to any significant degree. Notwithstanding the performance advantage LIBs hold over competing technologies, significant improvements to battery footprint, energy and power density, and cost can be achieved through technical improvements to electrodes that impart higher rate capability, higher charge capacity, and, in the case of cathodes, sufficiently high voltage. In this regard, new advances in materials need to be leveraged to usher in the next generation of the LIBs. Borrowing complex hierarchical structures found in nature, a superior approach might incorporate the use of hierarchical materials as the basis for the design of new electrodes, collectors, and separators in LIBs. This topic endeavors to develop the fundamentals of such a hierarchical structure design for improved electrochemical performance of LIBs.

For this exam, focus on the following…
Prepare a research and development proposal, per the instructions below, that if funded will allow you to ***develop a systematic methodology for the design of multidimensional, self-assembled, hierarchical structures for the cathode and anode of LIBs.*** The methodology should be guided by physico-electro-chemical, thermodynamic, and kinetic principles for optimizing the structures. Multidimensional porous structures of electrodes to facilitate rapid ion and electron transport pathways and short solid state diffusion lengths should be investigated. Design of porosity will be directed by accessibility of solvated ions in the electrolyte without compromising the tap density of electrodes. LIBs with prototype hierarchical electrodes will be fabricated and evaluated to verify the design approach and identify the optimization parameters and methods for practical implementation.

REFERENCES:
1. L. Zhou et al., "Recent Developments on and Prospects for Electrode Materials with Hierarchical Structures for Lithium-Ion Batteries," Advanced Energy Materials, 8, 1701415, (2018).
2. M.F. Rodrigues et al., "A materials perspective on Li-ion batteries at extreme temperatures," Nature Energy, 2, 17108 (2017).
3. H. Zhang et al., "Three-dimensional bicontinuous ultrafast-charge and -discharge bulk battery electrodes," Nature Nanotechnology, 6, 277 (2011).
4. ncbi.nlm.nih.gov/pmc/articles/PMC5430621

KEYWORDS: Li-ion batteries, Hierarchical materials, electrodes, collectors, separators

You are the Chief Technology Officer of a company that has specialized in creating low volume customized high reliability Li-ion based energy storage systems for specific applications in demanding environments. Your CEO believes that the company's expertise in micro to nanoscale Li-ion based energy storage materials, processing, and devices could provide a research and development path to meet DOD objectives in their solicitation. Your job is to define the research and development needed for new base technologies that would provide the platform for many future LIB technologies, and perhaps even expansion into other harsh environment markets (aircraft, spacecraft, etc.).

While meeting the DOD performance requirements are your priority, the cost of customized systems for LIB improvements will always be very high as compared to off the shelf commercial systems. In order to have potential to be competitive in other market applications which value compact, high-performance, it is desirable if your approach can be easily modified or adapted for lower price-point markets.

Your job as CTO is to deliver a complete proposal with your plan for the company to compete in this area to your CEO by your deadline.

YOUR DELIVERABLE

Your task is to write an internal proposal for your corporate officers describing your idea for research and development. The proposal should include the following:

- Executive summary (one page)
- Risk assessment roadmap form (one page)
- Full proposal (15 pages maximum)
- Appendix A: List of references (no page limit)
- Appendix B: Ranked list of intellectual property documents examined (no page limit)

Most Importantly – The significance and novelty of your creative solution, one that moves the boundaries of knowledge outward, will be the primary assessment focus of your review panel. The list below is just a minimum list of issues you might consider. There may be many more. The point is that your proposal ***should contain the evidence*** needed to make an effective and compelling case to your CEO in order to insure that she/he makes the right decision.

At a minimum, be sure you address all of the following:

Current Science and Technologies - What is already being done in this area by other researchers, companies and governmental institutions? Describe the current state-of-the-art for both the science and the implementation. Use diverse resources such as science literature, journals, conference proceedings, the internet, patents and other sources of existing public knowledge. ***Cite all references you use and use quotes for any word-for-word transfer to your report.***

Your Design Approach – What is the basis for your design approach to the problem? Why is your technology better than existing technologies? What technology attribute(s) make it likely to be selected by DOD? Address scientific *and* engineering aspects of these questions. Where relevant, consider: device size, weight and power (SWAP) requirements; materials of construction; critical components and considerations that comprise the complete device-level or subsystem-level solution; and what are the required prototyping and/or production methods, tools and costs? ***Even if you are not an expert in all of the technological areas required to bring the end-product to fruition, you should at least be able to intelligently discuss the other critical components, considerations and R&D requirements.***

Research & Development Plan - Describe a set of tasks and/or tests you will complete to demonstrate that your approach is effective and that your implementation of the solution is meritorious of further R&D. ***This is essentially your design of experiments. What are your objectives? What are the tasks required to achieve those objectives?*** Where applicable answer the following:

i) What are the key product specifications that you are targeting and how do they compare to the specifications of the existing solution(s) if any exist?

ii) What mathematical models and/or simulation constructs will you use to validate your approach, especially if prototyping and test trials are costly?

iii) What are the key dependent and independent variables that you must utilize and evaluate to confirm the proposed solution works?

Above all, be specific and detailed about the key tasks to confirm feasibility and validity of what you are proposing.

Cost Analysis – Identify cost and market issues that will impact the pricing strategy of the solution you have proposed. Identify Strengths, Weaknesses, Opportunities and Threats (SWOT) in the market place. If you are unfamiliar with the typical SWOT marketing analysis, I encourage you to 'google it'. Consider such things as: the major cost items that would impact the implementation; which elements of your implementation solution would be handled in-house versus externally-sourced; major risk elements that could drive up costs if the primary path item fails; costs of IP licensing needed, etc. Provide justification and/or reasoning behind your decisions. Estimate manufacturing cost for the total system as the technology reaches mature stage, so the marketing team can determine potential for penetrating other markets. Avoid subcontracting design, manufacture or assembly of any proprietary component outside the company, because the CEO is concerned with potential IP leakage.

Intellectual Property – In Appendix B, list in rank order of importance ***all*** commercial, academic, and governmental IP sources that were consulted while formulating the answer, including reference data. For instance, include the patent number; title; inventor name; and assignee name for a patent. Discuss the 3 most significant IP documents affecting your approach to your solution in the 15-page document. Compare strengths and weaknesses of these approaches relative to your own. Recommend how these IP threats should be handled.

Hint – Clearly state your hypothesized solution. Identify its innovation(s) and advantages relative to state of the art. Describe both existing data, and work needed to support each aspect of the hypothetical solution. Consider theoretical, fabrication, and characterization aspects: for each, identify software/equipment and methods to use, parameters to vary, anticipated outcomes, and possible alternatives in the event of unsatisfactory results. Discuss material, process, device, and systems aspects of your solution. *Refine* your hypothesized solution as you accumulate information and prepare the manuscript. **Remember**: clearly distinguish what is known from what is hypothesized or not known. What is needed to distinguish the important things to know?

Reference the 2020 PhD Candidacy Exam Guidelines document for general instructions.