Total Organic Redox Flow Batteries

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Introduction Renewable energy sources such as solar and wind could potentially transform America's energy landscape; however, the intermittent production of these power sources necessitates grid-scale energy storage solutions. Additionally, the American electric grid is currently unable to match supply to demand, employing redundant generators that mostly lie idle and producing excess, wasted power when demand is overestimated. Coupling energy storage systems to the grid would allow for renewable energy integration, balancing services, cold-start services, and emergency reserves [1,2]. Current energy storage systems are limited by cost and practicality, and progress in the field has been incremental at best. I propose that an investigation of redox flow batteries employing organic electrolytes, particularly electrolytes from biological systems, could yield a simple, cost-effective, and scalable solution to our energy-storage needs.

Redox flow batteries (RFBs) are a promising solution for grid-scale energy storage due to their customizability, scalability, efficiency, simple design, and cyclibility [1,2]. Despite these advantages, RFBs with aqueous electrolytes, the most heavily investigated type of RFB, are limited by low active species concentrations and a maximum operating voltage bounded by water electrolysis [3,4]. Organic RFBs have a larger operating voltage window, a larger temperature range, good kinetics, and easily-synthesized (as opposed to mined) electrolytes [4,5]. For this proposal, I plan on working under Dr. Fikile Brushett at the Massachusetts Institute of Technology, one of the first PIs to study total organic RFBs [4].

Objectives

1. **Characterize** and **simulate** desirable features of organic compounds for RFBs.
   Due to the wide variety of feasible organic electrolytes, efficient screening of potential organic compounds is imperative. A computational materials science approach could lead to the development of such a tool. The most pressing challenge in total organic RFB investigation is the identification of systems with higher concentrations of active species [4]. Therefore, I propose the development of a tool to quickly estimate the solubilities of complex organic compounds in organic solvents. Most advanced research in this area has been for pharmaceutical processing applications [6], but a similar functional-group based approach should lead to a simple yet sufficiently accurate model. After identification of the most promising organic and bioorganic solute/solvent pairs, I will prototype batteries with these compounds, thereby both refining the model's accuracy and uncovering additional characteristics of good organic electrolytes. Dr. Brushett's experience in organic RFB synthesis will be critical in the completion of this objective.

2. **Investigate** compounds from electron transport chains as RFB electrolyte candidates.
   Biological electron-transport chains (ETCs) are known to be one of the most efficient redox mechanisms known to mankind. Studying the features of these systems from the perspective

of RFB development could lead to critical insights into efficient redox reactions and even potential electrolytes. In particular, biological membranes are efficient and effective, whereas synthetic membranes are expensive or unsuitable. While quinones and their derivatives have been promoted and used in battery applications for some time [4,7], few other ETC compounds have been investigated. I propose a preliminary review of the ETC literature to parallel concepts and find electrolytes for battery development. This research will also lead to a better understanding of biological redox electrochemistry, which could have medicinal implications. The use of biology in batteries is not new to MIT; MIT faculty from various engineering departments have collaborated on novel biological electrode fabrication [8], demonstrating the interdisciplinary collaboration required for success in this endeavor.

3. **Collaborate** with JCESR and industrial partners to develop and commercialize RFBs.
   The DOE's Joint Center for Energy Storage Research (JCESR), headquartered at Argonne National Lab, is a consortia of universities, national laboratories, and battery companies tasked with rapid R&D of next-generation battery systems [9]. Working with JCESR will provide access to experienced battery researchers, advanced instrumentation, and supercomputer facilities. In particular, JCESR's electrolyte genome database of "soft" electrolytes lays the groundwork for our bioelectrochemical modeling [9]. Additionally, leading industrial battery companies such as Johnson Controls (JCESR member), General Electric, and Siemens have wide expertise in developing advanced batteries and smart grid technology. Capitalizing on industrial expertise in scale-up and manufacturing would focus our efforts on the most promising research avenues.

4. **Publicize** these results in both scientific and popular literature.
   As this technology could face the public, a key aim of this project is public exposure via publications, exhibitions, and demonstrations. The advantages of this technology are easily illustrated by comparing analogous features to those of combustion-powered automobiles (i.e. energy storage capacity is most easily increased by enlarging the fuel tank, as opposed to increasing the efficiency of the combustion engine or the gasoline). This technology also emphasizes the importance of science to all Americans, as successful implementations of organic RFBs could reduce carbon emissions and open-pit mining as well as America's dependence on foreign fossil fuels and rare earth metals.

References

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