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Title: Design of State-of-the-art Flow Cells for Energy Applications

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Intended for: Data sheet for LDRD funded project

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Project

20180710PRD1

Principal Investigator

Ping Yang

Title

N/A

Data Sheet. The following fields comprise the Project Data Sheet, the document upon which LASO concurrence is based.

Project Description (Limit 300 words):
Briefly describe the project and explain its cutting-edge, high-risk, high-potential science, technology, and/or engineering. Define all acronyms. Write in layman's terms.

The worldwide energy demand is increasing every day and it necessitates rational and efficient usage of renewable energy. Undoubtedly, utilization of renewable energy can address various environmental challenges. However, all current renewable energy resources (wind, solar, and hydroelectric power) are intermittent and fluctuating in their nature that raises an important question of introducing effective energy storage solutions. Utilization of redox flow cells (RFCs) has recently been recognized as a viable technology for large-scale energy storage and, hence, is well suited for integrating renewable energy and balancing electricity grids. In brief, RFC is an electrochemical storage device where energy is stored in chemical bonds, similar to a battery, but with reactants external to the cell. The state-of-the-art in flow cell technology uses an aqueous acidic electrolyte and simple metal redox couples. Thus, there is an urgent call to develop efficient (high-energy density) and low-cost RFCs to meet the efflorescent energy storage demands. To address the first challenge of achieving high-energy density, we plan to design and further modify complexes composed of bifunctional multidentate ligands and specific metal centers, capable of storing as many electrons as possible. In order to address the second challenge of reducing cost of the RFCs, we plan to use iron (Fe) metal as it regularly occupies multiple oxidation states and is the second most abundant metal in the earth ' s crust that makes it an ideal metal for improved energy densities, higher potentials, and numbers of electrons per molecule while maintaining potential cost competitiveness. Density functional theory calculations considering solvation effects will be performed to yield accurate predictions of redox potentials.

Tie to Missions (Limit 250 words):
Describe in narrative form the specific contribution your work makes to the missions identified on the Relevance page in Q, especially those with A relevance. Define all acronyms. Write in layman's terms.

The scientific results of the project will not only spark further experimental verification of the proposed redox flow cells, but will also be used as a general guideline towards the realization of novel inexpensive, safe, and high-performance flow cells, which could be implemented in the electricity grids in the near future. This project directly responds to the aim of approaching cost target on large-scale energy storage ($150/kWh) by Department of Energy, and Strategic Investment Plan on Energy Storage of Los Alamos National Lab. Having developed such systems, people will be able to effectively store and use greener electricity rather than relying on carbon energy sources, such as fossil fuels, which are in short supply.

Expected Results (Limit 100 words):
Summarize the overall technical goals of the project and the anticipated impact on the relevant science and/or engineering fields. Define all acronyms. Write in layman's terms.

The scientific results of the project will not only spark further experimental verification of the proposed RFCs, but will also be used as a guideline towards the realization of novel inexpensive, safe, and high-performance flow cells, which could be implemented in the electricity grids in the future. This project directly responds to the aim of approaching DOE ' s cost target on large-scale energy storage, $150/kWh, and LANL ' s Strategic Investment Plan on Energy Storage. Having developed such systems, people will be able to effectively store and use greener electricity rather than relying on carbon energy sources, which are in short supply.

Briefly describe the key accomplishments of your project during the past fiscal year:

Do not list publications, conference presentations, etc.
Instead, describe in narrative form, the tasks and goals accomplished during the past fiscal year.
These tasks should reflect those outlined in the Proposed Work section of last year's Data Sheet.

Define all acronyms. Write your information in layman's terms. This information may be used to assess whether or not there is sufficient evidence of progress to warrant continuation of the project.

Past Year's Accomplishments (for continuing projects only) (Limit 700 words):

N/A

Proposed Work: Tasks and Goals for the Next Fiscal Year (Limit 300 words):
Describe the tasks and goals to be accomplished in the next fiscal year. Provide sufficient details to help us evaluate the progress of the project. Define all acronyms. Write in layman's terms.

The overarching goal of Dr. Popov's project is to develop efficient (high-energy density) and low-cost flow cell batteries to meet the efflorescent energy storage demands. To address the first challenge, he plans to design and further modify complexes composed of bifunctional multidentate ligands and specific metal centers, capable of storing as many electrons as possible.
For the FY18, Dr. Popov will work on the single metal center (Fe) complexes to predict their electrochemical properties, such as reduction and oxidation potentials and their spectroscopic signatures.

Administrative Information. The following fields are used by the LDRD Program Office for administrative and reporting purposes.

Work Description (Limit 256 characters):
For reporting purposes, provide a brief, one- to two-sentence, description of the work of your project, targeting a lay audience. Limit: 256 characters.

This project is to develop efficient (high-energy density) and low-cost batteries to meet efflorescent energy storage demands.

Congressional Summary (Limit 200 words):
Briefly summarize the national security challenge the project will address, the high-level goals of the research, and the expected outcomes. State the impact the research could potentially have on DOE/NNSA missions. Write in layman's terms for a non-technical audience composed primarily of congressional stakeholders. Limit: 200 words.

The scientific results of this project will not only spark further experimental verification of the proposed redox flow cells, but will also be used as a general guideline towards the realization of novel inexpensive, safe, and high-performance flow cells, which could be implemented in electricity grids in the near future. This project directly responds to the aim of approaching DOE's cost target on large- scale energy storage, $150/kWh. Having developed such systems, people will be able to effectively store and use greener electricity rather than relying on carbon energy sources, such as fossil fuels, which the world will run out of sooner or later.

Transition Plan (Limit 500 words):
For an internal audience, 1) identify the Program Representative and the Division Leadership (DR's) or a cognizant individual (all other components) you are working with to transition project capabilities after your project ends. 2) List transition-related actions and goals. 3) Include your initial proposal "Transition Plan" or "Program Development Plan", if applicable. Limit 500 words.

This project will have great impacts on the renewal energy and general inorganic chemistry programs that span across T, MPA and, C divisions.

Transition related actions & goals:

- communicate the research results in a timely manner to program representatives
- make connections to experimental teams who are working on the related topics
- write up a BES, NE, or other external proposal based on the results

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