# Plan Overview

*A Data Management Plan created using DMPTool-Stage*

**Title:** CAREER: Probing Function in Paramagnetic Sodium Electrodes

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**Template:** NSF-DMR: Materials Research

**Project abstract:**

The proposed research seeks to answer the question: Can widely-applicable design criteria for next-generation cathode materials be obtained based on relations between composition, crystal structure and electrochemical properties?Specifically, the study aims to decouple and assess the effects of structure, the nature of the redox-active metal species and of the (poly)anion framework on alkali-ion conduction, on the rate of electron transfer and on the structural stability of a range of Na-ion cathode materials, including NASICON and alluaudite-type polyanion cathodes and weberite-type fluorides. Insights gained over the course of this work will allow the rational design of robust Na-ion host materials with predictable electrochemical properties, surpassing slower trial and error approaches. Educational activities will be aimed at students from diverse institutions around the country and will provide substantive experiences to increase the representation of minorities in STEM, while encouraging exchanges on the topic of energy sustainability. I will teach a series of online classes on methods for energy research, with a remote lab component. I will also organize a yearly 2-day symposium on diversity and sustainable energy, where students will present their work and explore research and policy questions related to sustainable energy. The success of these activities will be assessed based on a set of pre-defined criteria and documented through surveys and reports.

**Start date:** 12-31-2020

**End date:** 12-30-2025

**Last modified:** 08-03-2020

## CAREER: Probing Function in Paramagnetic Sodium Electrodes

Undergraduate and graduate students engaged in the research described herein are expected to coauthor peer-reviewed manuscripts in high-impact journals, including *Chemistry of Materials*, *Journal of Materials Chemistry A*, *Energy and Environmental Science* and *ACS Applied Energy Letters*. The supporting information accompanying these publications will include detailed experimental/simulation/synthetic procedures, as well as detailed information on models used for data analysis. All of the journals listed above make supporting information files publicly-available online free of charge.

Research results will also be disseminated via oral communication. Students will be trained to convey their results effectively and will be encouraged to participate in national conferences, such as Electrochemical Society (ECS), American Chemical Society (ACS) and Materials Research Society meetings, to deliver an oral or poster presentation.

Battery electrode material samples will be synthesized in powder and single crystal form and identified through a consistent and systematic labeling procedure, which will include: sample composition, name of researcher and date. Experimental data generated over the course of the research will include synthesis procedures and results from characterization of battery electrode samples. Digital characterization data (in tabular form) will be produced by solid-state NMR spectroscopy, X-ray and neutron diffraction, quasi-elastic neutron scattering, X-ray photoelectron and absorption spectroscopy, and Mössbauer spectroscopy. Additionally, analysis of neutron scattering data using the maximum entropy method will produce two- and three-dimensional plots of neutron scattering density. Rietveld refinements of scattering data will generate crystallographic data. Magnetometry will produce magnetic moment vs. temperature and vs. magnetic field datasets (in tabular form). Scanning electron microscopy will generate images. Electrochemical tests will produce voltage vs. capacity plots, as well as differential plots (in tabular form). Electrochemical impedance spectroscopy will generate Nyquist plots of the imaginary vs. real part of the impedance (in tabular form). Synthetic work and optimization of NMR experimental procedures will be documented in lab notebooks and generate physical data. First principles simulations will produce text files, density of states plots and two-dimensional charge density maps. Educational materials will be digitized.

In order to allow for interoperability, reproducibility, and reuse, all data will be stored and saved following standards and open formats. Experimental characterization data will be stored and saved as, e.g., ASCII, CSV, Word, Matlab and Python files. Microscope images will be stored as portable graphic files (.tif, .jpg or .png format). Crystallographic data will be reported in standard crystallographic information framework (*.cif) format to facilitate visualization and further analysis through widely available software tools (VESTA, cif2file, etc.). Crystallographic data for previously-unreported compounds/structures will be uploaded to the ICSD database. First principles simulation input and output files will be stored as rich text format (*.rtf) files for readability across many programs and platforms. The CRYSTAL code manual will be provided along CRYSTAL input/output data to allow for interpretation of variables. Both CRYSTAL and VASP manuals are also available online.

All publication pre-prints will be made freely available, along with supplementary information, on the UC eScholarship website.

Over the course of the project, digital data will be internally stored and shared for collaborative work on the UCSB-administered, Box platform with unlimited cloud storage. The privacy, security and intellectual property protection of data stored in this manner are guaranteed by the privacy policy and terms of service contract between University of California and Box.

As a means of making data accessible and searchable, data collected over the course of this project will be stored in the data repository Dryad. Dryad enables easy data upload and description, and creates digital object identifiers (DOIs) for each dataset to help manage long-term data sharing through digital organization. Dryad is free of charge for UCSB researchers and can be accessed using a personal ORCID.

All data will be stored in Dryad and will be available under a public domain, creative commons license (CC0). Note that while a personal ORCID is needed to deposit data in Dryad, no ORCID is required to search, find and download datasets.

Laboratory notebooks and samples will be retained for a minimum of 5 years following the conclusion of the program and will remain the property of UC Santa Barbara/will be kept on campus after students graduate. All digital data produced over the course of the project and stored on Box will be moved to Dryad after completion of the project for indefinite storage (>5 years).

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