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8-10-2021

Nickel Catalyzed Electrochemical C-C Cross-Coupling Reactions

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Recommended Citation

Liu, T. (2021). Nickel Catalyzed Electrochemical C-C Cross-Coupling Reactions. Utah State University. <https://doi.org/10.26078/PF14-YB42>

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DATA MANAGEMENT PLAN

1. Expected data of the Research

The data generated in the PI's group are composed of analytical and spectroscopic characterization and measurement of redox active molecules and their electrolyte solutions, solid-state battery electrodes and membranes, redox intermediates, and reaction products.

Raw data will be generated by lab equipment. The raw data are primarily numerical, including NMR spectra (proton and hetero-nuclear; one and two- dimensional), Raman, infra-red and UV-visible absorption spectra, X-ray diffraction patterns, XPS data, SEM data, cyclic voltammograms, bulk electrolysis spectra, electric and impedance spectra.

Secondary data will be produced through analysis of raw data, and will include spectroscopic plots, polarization curves, capacity curves, energy efficiency plots, coulombic efficiency plots, voltage efficiency plots, Tafel plots, and tabulated data.

Collaborative studies with the co-PI, Dr. Daniel Ess at Brigham Young University will produce theoretical calculation results. Proposed education activities will produce evaluation data.

Total data are expected to be less than 100 GB.

2. Data Format

A detailed description of date, instrument setup, experimental design, procedure, observation, and results of each experiment conducted in the PI's group is recorded in hardcopy notebooks. Instrument-generated electronic data, such as spectra and plots, are stored in hard copies as printouts and/or instrument outputs, in addition to electronic versions, such as ASCII codes, CSV files, MS Office documents, PDF files, or other data-appropriate formats (e.g., .dta for electrochemistry data). All data are indexed in the hardcopy notebooks as a part of the research narrative.

3. Access to Data and Data Sharing Practices and Policies

Data will be made available to the public through publications in scientific journals and poster/oral presentations at academic conferences/seminars. Generally, secondary data, such as tabulated data (theoretical calculations), images (.tif or .jpg) and crystallographic format files are included in the supplementary information of published materials. These data will be deposited according to each journal's requirements.

Data are not posted on a website or made available to the public via a database prior to publication. It is not anticipated that data will be deposited in databases that mine the published literature (e.g. PubChem, NIST Chemistry WebBook). In general, the PI will make the data available to an interested party if the data are not being held as confidential for intellectual property reasons. Data will be shared after consultation with, and according to, the guidance of USU's Office of Innovation and Commercialization Services.

4. Policies for Re-Use, Re-Distribution and Production of Derivatives

The PI does not post data on his group website or any other available venues for general access. Links to published work are made available on the group website, with no disclaimers or terms of use, as these are determined by the journal where the data are published.

5. Archiving of Data

All data generated in the PI's group are stored for at least three years beyond the end of any funding period. To protect and preserve electronic data, it is redundantly stored and backed up. Raw data is stored 1) on the computer on which it is generated, 2) on a secured hard drive which is backed up weekly, and 3) in Box.com, which is a cloud storage system used by Utah State University. Files stored in Box.com are backed up nightly at multiple sites. Box.com ensures data integrity, includes version control, is password controlled and encrypted.

Secondary data is stored on 1) the secured hard drive with weekly backups and 2) in Box.com. Lab Notebooks are scanned when the notebook is completed (i.e., filled with data). Electronic versions are stored on 1) the secured hard drive with weekly backups and 2) in Box.com. To protect against water and fire damage, all hardcopy laboratory notebooks, spectrum printouts, are stored in a room on elevated steel shelves in a room with fire-stop doors, separated from any research laboratory. All hardcopy laboratory notebooks from previous researchers in the PI's group are permanently stored in his faculty office. Physical samples are stored in fireproof cabinets.

The PI assumes responsibility for ensuring all data is backed up and that the terms of this data management plan are followed.