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Collaborative Research: Harnessing Mechanics for the Design of All-Solid-State Lithium Batteries

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Data Management Plan

1. Roles And Responsibilities

PI Wang will oversee the implementation of all aspects of the computational data management plan in Tasks 2, 3, and 4. PI Warren will oversee the implementation of all aspects of the experimental data management plan in Tasks 1 and 4. Adherence to the data management plan will be reviewed on a monthly basis by PIs Wang and Warren.

2. Expected Data

Computations: The proposed research will generate output files from atomic simulations for the LLZO-Li-Cu interaction in all-solid-state lithium batteries from VASP and LAMMPS. The output files include log files of system-level parameters and dump file of atomistic-level information (for LAMMPS) and electronic-level information (for VASP). The output files from LAMMPS and VASP are usually of GB size. They will be used in nanoscale mechanics modeling of Li plating and stripping and inform the continuum modeling. They can also be used by other interested people to validate our methods and results. After obtaining the output data from atomic simulations, we will then implement the continuum model into the finite element solver of FENICS. Input files in python and output ASCII files will be generated. Post-processing and analysis will be performed with MATLAB. Therefore, MATLAB script files (.m) will be generated.

Experiments: The following data types are expected to be generated during the proposed research: 1) Scanning transmission electron microscope (STEM) image files and corresponding energy dispersive X-ray spectroscopy (EDS) measurements; 2) Photographs, optical microscope images, and scanning electron microscopy (SEM) images of ASSLB cells; 3) Electrochemistry data obtained during charge-discharge testing and electrochemical impedance spectroscopy measurements of ASSLB cells; 4) SEM-picoindenter image and data files; 5) AFM image and data files; 6) Physical samples ASSLB cells and cell components, including sputter- and sol-gel-deposited LLZO thin films, nanostructure ASSLB anodes, and LLZO pellet disk electrodes before and after testing.
The above data will be collected using software programs (e.g. Gamry Framework and Gamry Echem Analyst software for electrochemistry measurements, Clarity software for Poseidon Select E-chip in-situ electrochemistry experiments, Gwyddion for AFM image analysis). Numerical data will be processed by creating graphs and tables that compare the results of different experiments. Image-based data (e.g. STEM and SEM images) will undergo minimal processing to maintain the integrity of the images. Quality assurance and control measures will include: 1) Reporting uncertainties in measurements whenever possible; 2) Running replicate tests to ensure repeatability of experimental measurements; 3) Conducting regular measurements of control samples to verify instrument performance.

2. Period Of Data Retention

All the research data will be stored in PI Wang, PI Warren and students' individual work computers. Besides, the data will also be stored in PIs' external hard drives (1-5 TB storage capacity). All the data will be retained for a minimum of 10 years upon the completion of the project. Data will be released to the public once after publication.

3. Data Formats And Metadata

As part of our DMP, the following contextual details (metadata) will be required for all experimental and simulation data collected during the course of the proposed research: date, researcher overseeing data collection, instruments used, and sample preparation conditions (as appropriate). These details will be attached to each data file or physical sample.

4. Data Dissemination And Policies For Public Access, Sharing And Publication Delays

Public release of data through journal publications, conference proceedings, and graduate student theses will occur immediately following data collection, analysis, and peer review by colleagues. They will also be available on Digital Commons at USU. Computer-format data will be saved on computers installed in the research labs where the data is being collected and on the University of Utah College of Engineering network file share. Primary and metadata will be made available to the public through email requests, with PIs' contact information given on each publication.

5. Data Storage And Preservation Of Access

Short-term data storage (0-3 years) - Data will be stored on laboratory and PI computers, with regular data backup (physical backup including secondary hard drives, and cloud storage backup) during the research project timeline. Physical samples will be stored in PI Warren's laboratory. Critical data will also be stored on networked servers in the College of Engineering at UU which are regularly backed up.
Long-term data storage (3-10 years) - Data will be stored as both physical and electronic copies (secondary, portable hard drives) at UU and USU. Research data will be archived in USpace (UU) and in Digital Commons (USU). Research data deposited in USpace (UU) and Digital Commons (USU) receive a persistent and non-breakable URL (reference URL), which can provide linking within the repository as well as out on the Web, including published research articles.

6. Other

No significant intellectual property issues involved with the acquisition of the data are anticipated. In the event that discoveries or inventions are made in direct connection with this data, access to the data will be granted upon request once appropriate invention disclosures and/or provisional patent filings are made. The data generated, stored and maintained in this proposed research will also subject to USU and UU's policy regarding data management, and intellectual property.