Degradation mechanism study of lithium-sulfur pouch cells based on electrodeposition

A Data Management Plan created using DMPonline.be

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Project abstract:

Lithium-sulfur batteries have emerged as a promising option for next-generation energy storage devices due to their high energy density and low cost. However, the two main obstacles for practical Li-S batteries are the notorious lithium polysulfide intermediate shuttle and the sluggish kinetics of sulfur cathodes, especially under lean electrolyte conditions. In this proposal, we propose a detailed plan to gain insight into the degradation mechanism based on electrodeposition by 1) quantifying the critical deposition concentration of lithium sulfide that leads to cathode catalysts deactivation; 2) controlling the nucleation and deposition orientation of lithium sulfide; 3) using this knowledge to solve the challenge issues in Li-S batteries; 4) analyzing the data obtained in Work Packages 1 and 2 comprehensively to reveal universal rules for structure-activity correlation. Firstly, we will explain why catalysts can be easily prepared by electrodeposition as cathode hosts, and others do not. Next, the key factors affecting catalysts' deactivation and cell degradation will be disclosed. Then, different types of metal catalysts with suitable particle sizes will be developed that are highly active and selective for Li-S pouch cells. Ultimately, extensive data analysis will be performed to visualize the data and discover generalized rules for structure-activity correlation.

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FWO DMP (Flemish Standard DMP)

1. Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

				Only for digital data	Only for digital data	Only for digital data	Only for physical data
Dataset Name	Description	New or reused	Digital or Physical	Digital Data Type	Digital Data format	Digital data volume (MB/GB/TB)	Physical volume
Electrodeposition data and electrochemical performance data	The electrochemical analysis data are obtained from an electrochemical workstation using electrochemical analysis techniques, e.g., cyclic voltammetry, impedance spectroscopy, chronoamperometry...Storage in electrochemical workstation and electrochemical test system	*Please choose from the following options:* Generate new data	*Please choose from the following options:* Digital	*Please choose from the following options:* Experimental	*Please choose from the following options:* txt	*Please choose from the following options:* <1GB	
Material characterizations	XRD, UV-vis, ICP, SEM, TEM, AFM images,	Generate new data	Digital	Experimental	txt	<100GB	
Physical samples	thin separator and applied in lithium-sulfur batteries		Physical	Experimental			>10 dm^3

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

I will not reuse existing data.

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

- No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, …)? If so, please comment per dataset or data type where appropriate.

- No

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/Data transfer agreements/ research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

2. Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g., in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, Codebook.tsv etc. where this information is recorded).

Electrodeposition will be performed in an electrochemical workstation in our lab, all digital data are created by the instruments automatically, and the used conditions are recorded as well. Software Nova will be used to collect and analyse data, we also record the detailed test parameters in notebooks which will be stored in our lab. In addition, all physical samples will be stored in the lab which are available to everyone with permission from us.

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

- No

In our communal workstation, everyone has a document with their name on it. In addition, a detailed description of the dataset, including its testing parameters, and testing purpose. So we can find our data easier.

3. Data storage & back-up during the research project

Where will the data be stored?

OneDrive (KU Leuven)
Large Volume Storage

How will the data be backed up?

Personal back-ups I make (specify below). The data will be moved to our own computer ASAP for backing up.
Standard back-up provided by KU Leuven ICTS for my storage solution.

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely.
If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.

- Yes

Our storage computer will be cleaned regularly to confirm enough storage capacity.

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

All the initial digital data will be stored in the lab computers. First, our lab can only be opened by authorized persons after being trained by the technician. Second, only the authorized person has the code to start the lab computers.

What are the expected costs for data storage and backup during the research project? How will these costs be covered?

All the costs for data storage are covered by the Department of Materials Engineering.

4. Data preservation after the end of the research project

Which data will be retained for at least five years (or longer, in agreement with other retention policies that are applicable) after the end of the project? In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).

Electrochemical performance data will be retained for 10 years. For [physical samples, the lab manager will collect physical samples (wasted batteries).

Where will these data be archived (stored and curated for the long-term)?

Large Volume Storage (longterm for large volumes)

What are the expected costs for data preservation during the expected retention period? How will these costs be covered?

The estimate costs for data preservation during the expected retention period is 200 euros which can be covered by the department or a research project.

5. Data sharing and reuse

Will the data (or part of the data) be made available for reuse after/during the project? In the comment section please explain per dataset or data type which data will be made available.

- Yes, in a restricted access repository (after approval, institutional access only, …)

All digital data are accessible with permission from us or the university. Some electrodeposition parameters can be reused after finishing the project.
The physical samples are available for everyone after finishing the project.

If access is restricted, please specify who will be able to access the data and under what conditions.

All digital data are accessible with permission from us or the university. Some electrodeposition parameters can be reused after finishing the project.
The physical samples are available for everyone after finishing the project.

Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)? Please explain in the comment section per dataset or data type where appropriate.

- Yes, Intellectual Property Rights

All data will not be accessible to the public until they get published. We will share the data with our collaborators or anyone who has our permission.

Where will the data be made available? If already known, please provide a repository per dataset or data type.

KU Leuven RDR (Research Data Repository)

When will the data be made available?

The experimental system still under exploration and upon publication of research results.

Which data usage licenses are you going to provide? If none, please explain why.

CC-BY 4.0 (data)
Data Transfer Agreement (restricted data)

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- No

What are the expected costs for data sharing? How will these costs be covered?

During the research project, there are no expected costs for data storage and backup, our lab already has computers for data storage.

6. Responsibilities

Who will manage data documentation and metadata during the research project?

Myself (Hui Pan) and my supervisor (Jan Fransaer)

Who will manage data storage and backup during the research project?

Myself (Hui Pan) and my supervisor (Jan Fransaer)

Who will manage data preservation and sharing?

Myself (Hui Pan) and my supervisor (Jan Fransaer)

Who will update and implement this DMP?

Myself (Hui Pan)