Plan Overview

A Data Management Plan created using DMPonline

Title: Novel materials and structural optimization for high temperature CO_2 utilization

Creator:HAODONG WU

Principal Investigator: HAODONG WU

Affiliation: University of St Andrews

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ORCID iD: 0009-0008-3758-6777

Project abstract:

In recent years, solid oxide electrolysis cells have emerged as a cutting-edge technology with a wide range of potential applications, such as hydrogen production and carbon dioxide recycling. It has been shown that electrochemical conversion of carbon dioxide at high temperatures through electrochemical reactions offers an effective strategy for mitigating carbon emissions, and SOECs have played a pivotal role in this development. The primary objective of this research is to significantly enhance the carbon dioxide reduction reaction performance of fuel electrodes through the synergistic integration of two pivotal surface modification approaches: impregnation and exsolution. Furthermore, this study is dedicated to exhaustively exploring the prospective mechanisms that might exist in the synergistic effect of these two approaches.

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Novel materials and structural optimization for high temperature CO2 utilization

Data Collection

What data will you collect or create?

The experimental data involved in this project is outlined as follows:

· **Data used for phase analysis**

#XRD (X-ray Diffraction) Data: The XRD data provides insights into the crystalline structure of materials by analyzing the diffraction patterns produced when X-rays interact with a sample. The data typically exists in the following formats: .xy file, .txt file, .raw file, .cif file and .dat file.

#EDS (Energy-Dispersive X-ray Spectroscopy) Data: The EDS data provides elemental composition information, helping identify and quantify the elements present in a sample.The data typically exists in the following formats: .pdf file and .csv file.

#XPS (X-ray Photoelectron Spectroscopy) Data: The XPS data provides valuable information about the chemical composition, oxidation states, and surface chemistry of materials. The data typically exists in the following formats: .txt file, .vgd file, .vgp file and .csv file.

#Raman (Raman Spectroscopy) Data: The Raman data provides insights into molecular vibrations, crystal structures, and chemical compositions of materials. The data typically exists in the following formats: .txt file, .wxd file and .csv file.

· **Data used for electrochemical analysis**

#OCV (Open Circuit Voltage) Data: The OCV data provides the voltage difference between the anode and cathode in solid oxide fuel cells when there is no current flowing between those two points. The data typically exists in the following formats: .txt file, .csv file and .xlsx file.

#EIS (Electrochemical Impedance Spectroscopy) Data: The EIS data involves the impedance of an electrochemical system across a range of frequencies. It provides various electrochemical processes occurring within the cell, including electrode reactions, ion transport, and polarization effects. The data typically exists in the following formats: .txt file, .csv file and .xlsx file.

#DRT (Distribution of Relaxation Time) Data: The DRT data involves studying the time constants associated with various electrochemical and transport processes within the electrochemical system. The data typically exists in the following formats: .txt file, .csv file and .xlsx file.

#LSV (Linear Sweep Voltammetry) Data: The LSV data provides valuable information about the electrochemical behavior of electrode materials. The data typically exists in the following formats: .txt file, .csv file and .xlsx file.

· **Data used for surface topography**

#SEM (Scanning Electron Microscope) Data: The SEM data provides detailed images of surfaces at high magnification, utilizing a scanning electron microscope. The data typically exists in the following formats: .tiff file, .jpg file and .bmp file.

#TEM (Transmission Electron Microscope) Data: The TEM data provides detailed information about the morphology, crystallography, and composition of samples. The data typically exists in the following formats: .tiff file and .dm3 file.

· **Others**

#Laser Particle Size Analysis Data: Laser particle size analysis data includes information about the distribution of particle sizes within a sample. The data typically exists in the following formats: .txt file.

#Viscosity Analysis Data: Viscosity analysis data includes information about the viscosity of a sample under different conditions and may be presented as a function of shear rate or concentration. The data typically exists in the following formats: .txt file.

Any newly created variables from the process of data management and analyses will be updated to this part.

How will the data be collected or created?

Data collection

The majority of raw data will be generated directly by the testing instruments, while some raw data may also be converted into easily readable formats (.pdf file, .txt file, .csv file, etc.) by data processing software. For instance, EDS data is often exported and presented in the form of PDF reports. Please note that this procedure should not compromise the integrity of the experimental data. And the experimental data will be transmitted using either portable hard drives or shared cloud storage platforms.

File naming

The data will be categorized either by time and data type. The title of the top-level folder should be something like 'year-month', 2023-09, for example. The second-level titles should indicate the data type, such as 'XRD', 'SEM', and so on. Simultaneously, the file names should include essential testing conditions, such as 'CO2_1.2V_EIS_900' (atmosphere_method_temperature). Repeated measurements of experiments should be annotated with a version number after the name, such as 'CO2_1.2V_EIS_900_2.0'.

Documentation and Metadata

What documentation and metadata will accompany the data?

The stored data consists of two parts: raw experimental data, and processed data. In most cases, raw data refers to data exported directly from testing instruments, retaining the original data format; while processed data, for the most part, is in .txt, .pdf or .csv format. The data use log will document all data-related activities. And dataset documentation will consist of electronic codebooks documenting the following information: (a) a description of the research methodology and sample, (b) a description of each specific data source, and (c) a brief description of the raw data.

Ethics and Legal Compliance

How will you manage any ethical issues?

This study does not involve any ethical or moral issues.

How will you manage copyright and Intellectual Property Rights (IPR) issues?

The ownership of all research data resides with the University of St Andrews. Nevertheless, the timing for the public dissemination of experimental data will be deferred. The availability of experimental data to the public will be scheduled subsequent to the article's publication. Prior to the release of this article, meticulous security measures will be upheld, ensuring the data's safekeeping at designated backup sites. The complete dataset is expected to be accessible after the study and all related publications are completed, and will remain accessible for long time after the data are made available publicly.

Storage and Backup

How will the data be stored and backed up during the research?

All experimental data will be meticulously safeguarded according to a triple-backup principle. This principle encompasses not only the preservation of data in its original storage locale but also its replication on a designated data processing computer, a dedicated external hard drive for archival purposes, and a shared network drive endorsed by the University of St Andrews. These three-tiered backups of experimental data will undergo real-time updates every two weeks to ensure data currency and integrity.

A comprehensive assessment reveals that the current storage capacity adequately accommodates the execution of this backup strategy. I will assume the role of the primary facilitator for this plan. In case of data impairment at any of the backup repositories, data restoration will be promptly initiated using the available storage segments designated for the corresponding backups, thereby ensuring the continuity and resilience of the data preservation framework.

How will you manage access and security?

The management of data storage, involving both external hard drives and computers, will be conducted with stringent security protocols in place. Additionally, access to the cloud storage, which houses the data, will be subject to meticulous control mechanisms. Specifically, access will be confined to individuals designated as project participants, who will possess the authority to view and retrieve the data as required by the project's scope and objectives.

Selection and Preservation

Which data are of long-term value and should be retained, shared, and/or preserved?

All chosen experimental data will be meticulously backed up, ensuring the long-term retention of data essential for supporting publication endeavors. Broadly, this data subset encompasses not only the evidence substantiating conclusions presented in research articles disseminated to the public, but also includes data that has yet to be comprehensively expounded upon. Data that has been confirmed to result from experimental errors will be excluded and subsequently destroyed.

What is the long-term preservation plan for the dataset?

An enduring strategy for data sharing and preservation will be implemented to ensure the data's accessibility and availability extend well beyond the project's duration. The principal approach to sustaining long-term data storage encompasses the utilization of cloud storage and the integration of solid-state hard drive backups. This comprehensive framework entails safeguarding the amassed data by securely housing and archiving it within the established cloud storage infrastructure provided by the University of St Andrews.

Data Sharing

How will you share the data?

Project participants will have access to the database via cloud storage, allowing them to retrieve data as needed. In addition, researchers within the same field will be granted access to this data segment after the publication of relevant articles.

Are any restrictions on data sharing required?

The overwhelming majority of experimental data will be shared in accordance with our commitment to transparency and open science. However, any data that remains unpublished or has yet to be verified for its accuracy will be withheld from public disclosure until such time as its validity can be confirmed.

Responsibilities and Resources

Who will be responsible for data management?

I will be directly responsible for overseeing the data management, and concurrently, my supervisors will shoulder the responsibility of supervising this process while also offering essential guidance and resources.

What resources will you require to deliver your plan?

I have already acquired and ensured the availability of the requisite resources to execute this plan. These resources primarily encompass the necessary hard drives and cloud storage solutions.