DMP title

Project Name Photocatalytic Valorization of Lignin towards Value-Added End Products - DMP title

Grant Title 12S1822N

Principal Investigator / Researcher Xuejiao Wu

Project Data Contact +32-485433295, wuxjxm@gmail.com

Description The project aims to develop a performant system with concrete potential for lignin valorization. Two successive processes will be pursued, which are depolymerization of lignin by concurrent cleavage of C-O and C-C bonds and upgrading of aromatic monomers from lignin depolymerization to biopolymers, both under the action of light. This project offers interdisciplinary research in bringing various research disciplines together including biorefinery, heterogeneous catalysis, photocatalysis, material science (CdS-based multifunctional catalysts and semiconductors with tunable redox potentials), chemical engineering (design of prototype flow reactor), and bioplastics (upgrading to produce biopolymer).

Institution KU Leuven

1. General Information

Name applicant

Xuejiao Wu

FWO Project Number & Title

12S1822N
Photocatalytic Valorization of Lignin towards Value-Added End Products

Affiliation

- KU Leuven

2. Data description

Will you generate/collect new data and/or make use of existing data?

- Generate new data

Describe in detail the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a table (see example) or as a data flow and per WP or objective of the project. If you reuse existing data, specify the source of these data. Distinguish data types (the kind of content) from data formats (the technical format).

The project includes two WP, i.e., Work Plan 1, photocatalytic depolymerization of lignin by concurrent C−O and C−C bond cleavage; Work Plan 2, photocatalytic upgrading of lignin-derived aromatic monomers to biopolymers. These two WP will both produce raw data and analyzed data. The following data types are expected:

Type of data	Format	Volume	How created
1. Catalyst performance testing data	.cdf	5-10 GB	The catalytic performance will be accessed by chromatography
2. X-ray diffraction spectrum, X-ray photoelectron spectrum, attenuated total refraction-infrared spectrum, X-ray absorption fine structure	uncompressed raw data	50-100 GB	Original characterization data
3. UV-vis diffuse reflectance spectrum, femtosecond transient absorption measurement	.txt	500 MB	Original spectral data
4. High-resolution scanning and transmission electron microscopy	.tif	50-100GB	Images will be taken by electron microscope
5. DFT results	uncompressed raw data, .tif, .txt, etc.	1-3 GB	DFT calculations will be performed by cooperators
6. Analyzed data	.opj	max 2 GB	Analyzed data by Origin Lab for a better understanding of the original results.
7. Analyzed data	.xls	max 2 GB	Analyzed data by Excel for a better understanding of the original results.

3. Legal and ethical issues

Will you use personal data? If so, shortly describe the kind of personal data you will use. Add the reference to your file in KU Leuven's Register of Data Processing for Research and Public Service Purposes (PRET application). Be aware that registering the fact that you process personal data is a legal obligation.

- No

Privacy Registry Reference:
Short description of the kind of personal data that will be used:

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, add the reference to the formal approval by the relevant ethical review committee(s)

- No

Does your work possibly result in research data with potential for tech transfer and valorisation? Will IP restrictions be claimed for the data you created? If so, for what data and which restrictions will be asserted?

- No

Do existing 3rd party agreements restrict dissemination or exploitation of the data you (re)use? If so, to what data do they relate and what restrictions are in place?

- No

4. Documentation and metadata

What documentation will be provided to enable reuse of the data collected/generated in this project?

1. The catalytic performance will be accessed by chromatography, which includes Gas Chromatography-Flame Ionization Detector (GC-FID), Gas Chromatography-Mass spectrum (GC-MS), High-Performance Liquid Chromatography (HPLC). The following information will be noted: catalyst, reaction conditions, reaction performing date. The information will be described in detail in a ReadMe file to describe corresponding data.
2. Characterization data including X-ray diffraction spectrum, X-ray photoelectron spectrum, attenuated total refraction-infrared spectrum, X-ray absorption fine structure will be saved in the original data formats. The data will be stored in separated folders according to different characterization methods. A ReadMe file in xls. will be created in every folder to describe the data, information will include the materials involved and the characterization conditions.
3. spectral data including UV-vis diffuse reflectance spectrum and femtosecond transient absorption measurement will be saved in txt formats first. The data will be stored in separated folders according to different characterization methods. A ReadMe file in xls. will be created in every folder to describe the data, information will include the materials involved and the characterization conditions.
4. High-resolution scanning and transmission electron microscopy will be applied to verify the successful synthesis of catalysts. The following information will be noted: dimensions, image type, bit-depth, pixel sizes, and microscope settings. The methodology and protocol will be described in detail in the lab book. A ReadMe file of the image collection will be written.
5. Cooperation with experts for DFT calculations is expected to declare the reaction mechanisms on the molecular level. The generated data including uncompressed raw data, .tif, .txt, etc. will be provided by the cooperator. These data will be put in order according to their types and a .txt file explaining these data will be put in the same folder.
6. Characterization data and part of the catalytic performance data will be analyzed by Origin Lab for a better understanding of the original results. A ReadMe file of the analyzed data will be written.
7. The majority of catalytic performance data will be analyzed in excel for better comparison. A ReadMe file of the analyzed data will be written.

Will a metadata standard be used? If so, describe in detail which standard will be used. If no, state in detail which metadata will be created to make the data easy/easier to find and reuse.

- No

The 7 types of data will be deposited in 7 folders, each of them contains a ReadMe file (.txt or .xls), so the data can be easily found and reused. At the end of this project, the 7 folders will be put in one folder, and an extra ReadMe file (.txt) will be generated to explain and summarize the 7 types of data in detail.

5. Data storage and backup during the FWO project

Where will the data be stored?

1. The majority of data will be kept on our research unit central storage facility. Copies can be made and kept on personal devices, including the hard drives and computers of the researcher (Xuejiao Wu) and of the lab.
2. Since we will collaborate with researchers (for characterization and DFT calculations) from other research units and groups, we will use OneDrive for active use of the data during the project.

How is backup of the data provided?

The data will be stored on the university's central servers and OneDrive with automatic daily back-up procedures.

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

The data will be stored on the university's central servers (e.g., KU Leuven long-term storage, cloud server, and Libary Archiv) with automatic back-up procedures, and the storage & backup capacity is sufficient.

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

The cost will be covered by the research group and partly from the current FWO bench fee.

Data security: how will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

The data will be stored in the university's secure environment, and can only be accessed or modified by authorized persons.

6. Data preservation after the FWO project

Which data will be retained for the expected 5 year period after the end of the project? In case only a selection of the data can/will be preserved, clearly state the reasons for this (legal or contractual restrictions, physical preservation issues, ...).

All data will be retained for at least 5 year period after the end of the project.

Where will the data be archived (= stored for the longer term)?

1. The data will be stored on the university's central servers (with automatic backup procedures) for at least 10 years, conform the KU Leuven RDM policy.
2. Our project will generate a large volume of data, some of which (like High-resolution scanning and transmission electron microscopy) may not be appropriate for sharing since it involves a small sample that is not representative. The investigators will work with the staff of the KU Leuven Libraries to determine what to archive.

What are the expected costs for data preservation during the retention period of 5 years? How will the costs be covered?

All data together will be compiled into one .zip document. This .zip document with a size < 300 GB will be hosed on the servers of KU Leuven. The storage is free of cost. The cost for support will be covered by the research group working budget.

7. Data sharing and reuse

Are there any factors restricting or preventing the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

- Yes. Specify:

All data were restricted for sharing before the publication of papers.

Which data will be made available after the end of the project?

Relevant data will be uploaded to KU Leuven Research Data Repository once an accompanying paper is published.

Where/how will the data be made available for reuse?

Relevant data will be uploaded to KU Leuven Research Data Repository once an accompanying paper is published. Data will be available on request.

When will the data be made available?

- Immediately after the end of the project
- Upon publication of the research results

Most data will be available after the end of the project. Some data obtained by 3rd party (e.g. DFT calculations and advanced photoelectric characterizations) will be available only after the publication of the research results.

Who will be able to access the data and under what conditions?

The created data will be available to anyone, provided that they give appropriate credit to the creators.

What are the expected costs for data sharing? How will the costs be covered?
N/A

8. Responsibilities

Who will be responsible for data documentation & metadata?
The investigator, Xuejiao Wu, will be responsible for the data documentation & metadata.

Who will be responsible for data storage & back up during the project?
The investigator, Xuejiao Wu, will be responsible for data storage & backup during the project.

Who will be responsible for ensuring data preservation and reuse ?
The investigator, Xuejiao Wu, and the PI will be responsible for ensuring data preservation and reuse.

Who bears the end responsibility for updating & implementing this DMP?
The PI bears the end responsibility of updating & implementing this DMP.