Data Management Plan (DMP)

Project name: Understanding Flexibility in Responsive Metal-Organic Frameworks (MOFs) (MOFFLEX)

Project code: 12E5123N

Fellow Researcher: Jesus Gandara Loe

Supervisor: Rob Ameloot

Project Data Contact: jesus.gandaraloe@kuleuven.be

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Project description: Adsorption-based separation is a key step to obtain high-purity compounds in the chemical industry. Metal-organic frameworks (MOFs) are a promising group of porous adsorbents characterised by their high adsorption capacity. Unlike in most all-inorganic adsorbents, structural flexibility has been observed in certain MOFs. Most research has been devoted to exploring and understanding the structural changes in extremely flexible structures that display very large changes in their unit cells. Despite this focus on a small subset of very flexible materials, almost all MOFs are flexible to some degree. As a result, the adsorption of molecules larger than the crystallographic pore window is commonly observed. Despite its obvious relevance, flexibility is understudied in most MOFs, and its effect in adsorption and separation remains unknown.

MOFFlex aims to observe and understand adsorption-induced flexibility in different classes of MOFs that thus far remain understudied in this context. In addition, the effect of the MOF particle size and the presence of polymer binders on the framework flexibility will be systematically analysed. To this end, MOFFLex will combine an extensive toolbox of diffraction and spectroscopic in-situ techniques (both in the lab and at synchrotron facilities), in-depth structural characterisation, and the controlled synthesis of MOF particles and composites. A series of aliphatic alcohols will be used as probe molecules with practical relevance.

Institution: KU Leuven

1. GENERAL INFORMATION

Name of the Applicant

Jesus Gandara Loe

Project Number & Title

12E5123N **-** Understanding Flexibility in Responsive Metal-Organic Frameworks (MOFs) (MOFFLEX)

Affiliation

KU Leuven

2. DATA DESCRIPTION

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

Describe the origin, type and format of the data (per dataset) and its (estimated) volume, ideally per objective or WP of the project. You might consider using the table in the guidance.

Objective 1 (**O1**): **Design of synthesis procedures to control the crystal size of class 2 & 3 MOFs**. This objective will require the development and optimisation of procedures based on the addition of modulators in microwave-assisted solvothermal synthesis.

Equipment	Raw format	Exported format
X-ray diffraction	XRDML	CSV
Adsorption 3flex equipment	.XLS	CSV
Scanning electron microscope	TIF	

Objective 2 (**O2**): **Evaluation of the effect of flexibility in adsorptive separation processes through adsorption measurements and high-resolution in-situ techniques.** This objective will require the combination of single-component and multi-component adsorption measurements of alcohols and in-situ PXRD, LF-NMR, and IR measurements to evaluate the interactions and changes upon guest adsorption.

Equipment	Raw format	Exported format
X-ray diffraction	XRDML	CSV
FTIR spectrometer	XLS	CSV
LF-NMR	TIF	
Adsorption 3flex equipment	XLS	CSV

Objective 3 (**O3**): **Elucidation of the effect of polymer-MOF interactions to optimise the selection of polymer binders for MOF shaping**. This objective will require an in-depth understanding of the interactions between polymer binders and controlled-size MOFs.

Equipment	Raw format	Exported format
Synchrotron X-ray diffraction	XRDML	CSV
Adsorption 3flex equipment	XLS	CSV

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 your host institution's privacy register - not relevant yet)

- No

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?

- An overview file that contains references to the raw data files will be kept. Regular reports based on the data will be generated using Microsoft Word. PowerPoint files will be used for presentation at regular internal meetings between the WP leaders and researchers involved in the project. In both the Word reports and Powerpoint presentations, the file names of the raw data files will be included.

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 details of each experiment will be kept in an electronic lab notebook. In this notebook, also the names of the raw and processed data files will be mentioned. Files will be named according to a pre-agreed convention. This working method obviates the need for a separate INFO.txt file in each directory yet ensures that the data can be understood by other team members and can be reused in the future.
For published papers, the subset of the raw and processed data discussed in that manuscript will be copied and organized according to the paper structure. Likely, this is the data subset that will be most frequently revisited and shared afterward.

5. DATA STORAGE & BACK UP DURING THE PROJECT

Where will the data be stored?

- The data will be stored via a cloud storage solution that allows sharing with the researchers involved in the project.

How is backup of the data provided?

- The data on the cloud storage server are automatically backed up. Unlimited versioning is included in the selected plan so that accidental erasing or modifying does not pose a risk.

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 total amount of data generated during the project should not exceed a few TB and is therefore compatible with the selected cloud storage solution.

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

- The costs for saving the data to the cloud storage server (including regular backup) should not exceed a few hundred euros. These costs will be covered by the project.

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

- The data generated during the project will be systematically transferred to the cloud storage server. Only the WP leaders and researchers involved in this project will have access to the shared folders where the data, reports and presentations will be stored.

6. DATA PRESERVATION AFTER THE 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 the generated data will be stored on the cloud storage server for a period of 5 years after the end of the project.

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

All the generated data will be stored on the cloud storage server for a period of 5 years after the end of the project.

Beyond 5 years after the end of the project, one of the following options will be picked (1) continuation of storing the data on the cloud storage server or (2) transferring the data to the KU Leuven central servers for archiving.

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

The annual cost for long-term storage of the data, either through a cloud storage service or the university's central servers, is estimated at a few hundred euro. Since the budget of the current project will no longer be available, creative solutions will have to be found

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)?

- No

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

- In case no restrictions apply, the written reports and Powerpoint presentations summarizing the results obtained can be made available. The (raw) data used in publications can be made available on a repository, if e.g. requested by the Editors or Publisher of a scientific journal.

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

- Upon request by email

The data that will not have been uploaded in a resository such as 'Scientific data' (https://www.nature.com/sdata/) to accompany a publication can be requested via email.

When will the data be made available?

- Upon publication of the research results

Description of the full scientific method and results will be made available with journal publications.

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

Upon request, access to the samples and data can be granted, upon agreement of the project leaders. Commercial reuse will not be allowed.

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

Because of the choice for a cloud storage solution for the data, no additional costs will be booked for data sharing.

8. RESPONSIBILITIES

Who will be responsible for data documentation & metadata?

The project leaders and the researchers involved in this project will be jointly responsible.

Who will be responsible for data storage & back up during the project?

The project leaders and the researchers involved in this project will be jointly responsible. Because of the choice for a cloud storage solution, no additional action is needed for data backup.

Who will be responsible for ensuring data preservation and reuse?

The project leaders and the researchers involved in this project will be jointly responsible.

Who bears the end responsibility for updating & implementing this DMP?

The project leaders bear the end responsibility of updating & implementing this DMP.