
Junior postdoc FWO number 12ZS623N

A Data Management Plan created using DMPonline.be

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Template: FWO DMP (Flemish Standard DMP)

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Project abstract:

A technological revolution is often based on the discovery of novel materials, graphene being one of the most popular of such materials. Another class of famed materials comprise of the so-called twodimensional covalent organic frameworks (2D-COFs). These frameworks are ultra-thin (one-molecule thick), complex, sheet-like macromolecules that can be synthesized in a truly bottom-up approach and have fascinating applications in fields like advanced electronics and catalysis. Metal containing 2D-COFs have recently shown to possess great potential as electrocatalysts for CO₂ fixation and its conversion into value added chemicals. This project pushes the state-of-the-art by carrying out the on-surface synthesis, the realtime, real-space single molecular level characterization of structurally precise, heteroatom-rich and stable metal containing 2D-COFs followed by the evaluation of their stability and surface dynamics after long exposures to reductive potentials in well-controlled CO₂ operando experiments. By working at reduced dimensionality, this project aims to extract crucial structure-property relationships which will guide the design of the future electrocatalytic frameworks.

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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
S1	Experimental STM-AFM and EC data	<i>Please choose from the following options:</i> Generate new data	<i>Please choose from the following options:</i> Digital	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Experimental 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> .xml, .tab, .csv, .pdf, .txt, .jpg 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <50TB 	
S2	Modeling data	<i>Please choose from the following options:</i> Generate new data	<i>Please choose from the following options:</i> Digital	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Simulations 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> .mat 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <1TB 	

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:

N/A

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).

All collected data will be labelled for each experiment and a table with a summary for every experiment will be provided. This table contains: date at which data was acquired, sample description (name/s of compound/s, concentration/s, ratios and labelling, substrate types), measurement parameters (Type and model of Instrument), report of results and short conclusion, suggestion towards follow-up experiment. Further, a detailed description of the used protocol to prepare the samples (for both successful as well as unsuccessful results) will be written and kept in the electronic lab journal with regular backups.

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 metadata standard will be used. Necessary documentations on the creation of the data will be include in the same folder with the dataset:

Metadata generated automatically by the measurement setup, and is embedded in the microscopy/electrochemical data.

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

Where will the data be stored?

The data is stored on personal portable hard drives as well as each equipemnt used to take such data. Also cloud storage service "one drive" and KUL personnel's internet drives offered by KU Leuven.

The accepted version of the final manuscripts (+ accessory datasets and supporting information) are submitted in open access journals and in the KU Leuven library's depository. In addition, relevant data will be transferred to the self-mirrored long-term storage capacity by the KUL ICTS for long-term storage till at least 5 years after the project

How will the data be backed up?

The data will be backed-up automatically for remote data storage on a daily basis in the cloud using one-drive storage. Additionally, other copies of the data will be kept at different physical locations using portable hard drives

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

Storage and backup capacity is already present. In any case it can be extended further by purchasing additional portable hard drives or cloud data volumes.

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

Access to the data is restricted by online build-in safe logins and by physical restriction of access to the portable hard drives through the security system installed in the building of the affiliation.

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

Expected additional costs remain limited, as data storage is ensured.

Additional costs may include the purchasing of further portable hard drives (2TB for 169euro), which will then be covered by the personal bench fee. Cloud-based data storage using one drive software volume will be shared with the host research group.

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...).

Only a selection of relevant data will be preserved. Selection of data destined for long-term storage will be assessed by the applicant and the promoter on a yearly basis. Naturally, all data and metadata used/linked to published articles, will be preserved in the university library depository.

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

The selected data will be stored on the university's central servers for at least 10 years, confirm the KU Leuven RDM policy. In addition, the selected data will be preserved on minimum 3 different portable hard drives which are kept locked at different locations under the supervision of the promoter.

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

Costs for the retention of data on portable hard drives is already (partially)made. A total volume of less than 5TB is anticipated, that will result in a cost of approximately 1000 euro to be covered from the bench fee of this grant.

The storage has been set up for the research group, the shared cost will depend on the actual data generated from this 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, ...)

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

Requests to access the data can be made via email to the promotor or Postdoc, who will decide upon this request after consultation with the promotor and co-authors of articles and after the possible receiver has signed a data sharing agreement.

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

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

The data will be available physically and 'in-cloud' on

When will the data be made available?

Upon request to myself or PI via email as well as upon publication of research results.

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

Upon proper and agreement request all the data licenses will be provided.

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.

- Yes

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

Cost will be held by KU Leuven and/or host group.

Cost of sharing physical data will be covered my personal bench fee.

6. Responsibilities

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

Nicolas Arisnabarreta and Steven De Feyter

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

Nicolas Arisnabarreta

Who will manage data preservation and sharing?

Nicolas Arisnabarreta and Steven De Feyter

Who will update and implement this DMP?

Nicolas Arisnabarreta

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Application DMP

Questionnaire

Describe the datatypes (surveys, sequences, manuscripts, objects ...) the research will collect and/or generate and /or (re)use. (use up to 700 characters)

In this project, the data will be collected using different techniques and the generated data strongly depends on the individual tools:

1. Visualization of 2D M-COFs (.Par, .mi, .ibw – SPM)
2. Chemical nature characterization (Text US-ASCII – XPS)
3. Electrochemical methods (Text US-ASCII)

Whenever possible, the dataset will be made available online using the following formats:

1. Text content (.pdf.docx, .xls, .pptx, .);
2. Graphic content (.jpg, .png, .svg .tif,)
3. Video content (.avi, .mp4)
4. Modeling data (.mat)

Specific extension of all files will be converted to widely accessible formats of .jpg, .tif etc.

Specify in which way the following provisions are in place in order to preserve the data during and at least 5 years after the end of the research? Motivate your answer. (use up to 700 characters)

1. Designation of responsible person: Researcher and principal investigator (PI) (Dr. N. Arisnabarreta and Prof. S. De Feyter)
 - a. b.
2. Storage capacity/repository: The size of the data generated is not expected to be more than 2TB. The research group has already procured devices for regular storage and back up.
 - during the research: During the implementation of the project, data will be stored on the respective instruments as well as PI computer, which is backed up according to the internal regulations in university servers.
 - after the research: After the end of the research, samples and raw data must be stored for a minimum of 5 years. If inventions are made in connection data, access to data will be restricted until provisional patent filings are made according to the university agreement.

What's the reason why you wish to deviate from the principle of preservation of data and of the minimum preservation term of 5 years? (max. 700 characters)

N/A

Are there issues concerning research data indicated in the ethics questionnaire of this application form? Which specific security measures do those data require? (use up to 700 characters)

N/A

Which other issues related to the data management are relevant to mention? (use up to 700 characters)

N/A

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DPIA

DPIA

Have you performed a DPIA for the personal data processing activities for this project?

- Not applicable

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GDPR

Have you registered personal data processing activities for this project?

- Not applicable