# Paired electrocatalytic alkane dehydrogenation and CO2 reduction in a multicompartment electroreactor using metal-organic framework based proton conducting membranes

*A Data Management Plan created using DMPonline.be*

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**Template:** FWO DMP (Flemish Standard DMP)

**Principal Investigator:** n.n. n.n.

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**Project abstract:**

Alkane dehydrogenation is a central reaction not only in current chemical industry, but also in the revalorization of polyolefin waste feedstock. Dehydrogenation is endothermic and at high temperature (> 500°C) faces selectivity challenges. Here we will dehydrogenate alkanes at moderate temperature (100-200 °C), by driving the reaction with (renewable) electricity in a two-compartment electrochemical reactor. At the anode, we use either a noble metal catalyst that is promoted to enhance its selectivity for monodehydrogenation; or a homogeneous pincer Ir catalyst is used, which after alkane dehydrogenation and metal dihydride formation is regenerated at the anode. Ir pincers allow unique, e.g. terminal selectivity. At the cathode, the protons and electrons from the alkane are used to reduce CO2 to formic acid on modified Sn electrodes, which need to operate at the same temperatures as the anodic compartment. Critical is the membrane between anodic and cathodic compartments which must conduct protons even at 100-200°C; mixed matrix membranes with stable polymers (e.g. polybenzimidazole) and metal-organic framework fillers will be designed and applied. All compounds are assembled in a masstransport optimized electroreactor. Advanced operando techniques (in situ TEM, XRD, DEMS) are applied to characterize the catalyst in the actual reaction conditions, and to measure rates of dehydrogenation, proton transport and CO2 reduction.

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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)**

Procedures for performing reactions, for synthesizing electrocatalysts, for constructing setups and initial observations of these experiments will be gathered.
Such procedures will also result in raw data files containing chromatographic data (GC-FID, GC-MS, FTIR) and material characterization data (XRD, physisorption and chemisorption data or spectroscopic analysis via UV-Vis, NMR etc.).
These will be processed in excel files, summaries and presentations, finally culminating in manuscripts and/or patents. The combined virtual volume of these datasets will be limited (< 10 GB), and will consist mostly of data files containing GC chromatograms (up to 5 GB)

**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)**

The responsible person is Dirk De Vos (PI).
Physical hand-notes of procedures and initial observations are kept in lab books. Digital data, with unambiguous identifiers for reactions and materials, are kept in cloud storage from ‘Box’. KU Leuven offers an Enterprise Box account 3, which offers an easy and secure storage space of up to 100 GB for each user.

**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)**

not applicable.

**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)**

No.

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

Not applicable.

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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 |
|---|---|---|---|---|---|---|---|
| | Description | New or reused | Digital or Physical | Digital Data Type | Digital Data format | Digital data volume (MB/GB/TB) | Physical volume |
| | XRD patterns | *New* | *Digital* | *compiled* | *.xrdml* | 20 kB | none |
| | GC chromatograms | New | Digital | raw | .gcd | < 2Mb | none |
| | NMR spectra | New | Digital | processed | variable | 256 kB | none |
| | FTIR | New | Digital | processed | variable | 128 kB | none |
| | | | | | | | |

**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:**

not applicable

**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).**

Details to reproduce reaction procedures are described in a personal lab booklet. Upon presentation or publication of data, procedures are described in sufficient detail to enable a reproduction of the generated results for an experienced user. ReadMe-files or recording methods for advanced characterization are stored in parallel with generated data.

**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

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

**Where will the data be stored?**

Physical hand-notes of procedures and initial observations are kept in lab books. Digital data, with unambiguous identifiers for reactions and materials, are kept in cloud storage from ‘Box’. KU Leuven offers an Enterprise Box account 3, which offers an easy and secure storage space of up to 100 GB for each user

**How will the data be backed up?**

By using the cloud storage of ‘Box’, digital data will be stored in parallel on the cloud and on the personal computer of the applicant, guaranteeing back-up for this data. Most raw data is also stored and frequently backed up off-line on external 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

**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 for private data. An Enterprise Box account 3 for cloud storage ensures a secure environment.

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

The high capacity of the available external hard drive (1 TB) enables the preservation of data from multiple terminated or finished projects. Currently, an average of 15 GB is used for the finished projects of each user, which allows to divide its cost over approximately 60 users. Given the cost of the available hard drive of 120 EUR, the expected costs are negligible. The involved IT-expenses are included in the project’s consumable expenses or covered by reserve funds.

## 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...).**

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

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

Upon termination of the contract, the data will be transferred and stored on an external hard drive (Samsung Portable SSD T5 1 TB), managed by Annelies Van Vlasselaer.

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

The high capacity of the available external hard drive (1 TB) enables the preservation of data from multiple terminated or finished projects. Currently, an average of 15 GB is used for the finished projects of each user, which allows to divide its cost over approximately 60 users. Given the cost of the available hard drive of 120 EUR, the expected costs are negligible. The involved IT-expenses are included in the project’s consumable expenses or covered by reserve funds.

## 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.**

- No (closed access)

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

Upon request to the PI.

**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.**

- No

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

Upon request by mail

**When will the data be made available?**

Upon publication of the research results

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

none.

**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?**

No additional costs are expected as the data can be shared via online platforms (e.g. WeTransfer) or the already budgeted storage cloud from Box. If additional costs would occur they will be covered from reserve funds.

## 6. Responsibilities

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

Dirk De Vos and Annelies VanVlasselaer

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

Dirk De Vos and Annelies VanVlasselaer

**Who will manage data preservation and sharing?**

Dirk De Vos and Annelies VanVlasselaer

**Who will update and implement this DMP?**

Dirk De Vos and Annelies VanVlasselaer

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# GDPR

## GDPR

**Have you registered personal data processing activities for this project?**

- Not applicable

# Paired electrocatalytic alkane dehydrogenation and CO2 reduction in a multicompartment electroreactor using metal-organic framework based proton conducting membranes
# DPIA

## DPIA

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

- Not applicable