Scalable performant solar cell module for CO2 Reduction Coupled with Organic Synthesis

A Data Management Plan created using DMPonline.be

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Project abstract:

Sustainable synthesis of fuels and chemicals from CO2 can be achieved by mimicking the light-harvesting and catalytic processes occurring in plants. A viable artificial photosynthesis (AP) process is a grand challenge of scientific research, since it would not only alleviate the effects of global warming but would also create an alternative solar, chemical, and energy industry. Prior works predominantly focused on developing lightsensitive materials that can harvest solar light to excite the non-reactive CO2 molecules. Although this effort was on point, it was not sufficient for a lucrative AP process. Recently, a more holistic approach for AP systems has been introduced, not only considering thebmaterials but also studying the whole device and process design. This project aims to realize a breakthrough step in AP by designing and manufacturing a new type of lightharvesting panel based on honeycomb-like repetitive structures using low-cost materials. These panels will improve the light-harvesting efficiency of the existing light-sensitive
materials by increasing the active surface area and the efficient distribution of reagents. Moreover, to make the best of sunlight energy and achieve maximum output, we suggest
replacing the sluggish water oxidation reaction with value-added organic molecules transformation which will open a new horizon to provide additional economic value from the products The project aims to demonstrate the proof of concept with a complete scalable processing unit.

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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.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: ***N****(ew data) or* ***E****(xisting data)*	Indicate: **D**(igital) or **P**(hysical)	Indicate: **A**udiovisual **I**mages **S**ound **N**umerical **T**extual **M**odel **SO**ftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
Photo	Light irradiation experiments	N	D	N	xlsx	<100GB	NA
Electro	Electrochemical experiments	N	D	N	xlsx	<100GB	NA
Photoelectro	Photoelectrochemical experiments	N	D	N	xlsx	<100GB	NA
Ceramic	Ceramic experimental data	N	D	I,T	image, xlsx	<1TB	NA
Model	Photo/flow simulations	N	D	M	mph - COMSOL file format	<5TB	NA

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)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- 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.

- Yes

Prototype is evaluated (Photoelectro data) using space-time-yield as benchmark. This data will prove if there is exploitation chance.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or 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

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).

Each dataset will be stored with a standard readme files explaining which data is associated which publication, thesis chapter, patent. This is currently being developed by the PhD student Tobias El-Chalid, supervised by Prof. Leblebici.

Will a metadata standard be used to make it easier to find and reuse the data?
If so, please specify which metadata standard will be used.

If not, please specify which metadata will be created to make the data easier to find and reuse.

- Yes

Our most critical data, if not exploited will be uploaded to KUL RDR and EngrXiv and will be cited with own DOI.

Data Storage & Back-up during the Research Project

Where will the data be stored?

- Shared network drive (J-drive)
- OneDrive (KU Leuven)

Prof. Leblebici is the responsible from the 100+TB CIPT repository (being purchased) The short-term storage is the KU Leuven One-Drive. The long term is the CIPT repository.
This will be communicated in the following progress meeting.

How will the data be backed up?

- Other (specify below)

CIPT repository is backed up RAID5.

Is there currently sufficient storage & backup capacity during the project?

If no or insufficient storage or backup capacities are available, 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?

Only Prof. Leblebici gives and takes usage rights to the CIPT repository.

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

The CIPT repository (10kEur) is being purchased by multiple project budgets.

Data Preservation after the end of the Research Project

Which data will be retained for 10 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 preserved for 10 years according to KU Leuven RDM policy

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

- Large Volume Storage (longterm for large volumes)
- KU Leuven RDR

The CIPT repository is large enough and can be expanded. We calculate the cost of SPROUT data in 10 years will be roughly 2k Eur. Will be paid by the project budget.

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

See above please. 2kEuros.

Data Sharing and Reuse

Will the data (or part of the data) be made available for reuse after/during the project?
Please explain per dataset or data type which data will be made available.

- Yes, as open data
- Yes, as embargoed data (temporary restriction)

- Yes, as restricted data (upon approval, or institutional access only)

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

Prof. Leblebici
Prof. Vleugels

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 per dataset or data type where appropriate.

- Yes, intellectual property rights

As discussed in exploitation plans. The performance data will firstly be evaluated for exploitation. Tha data can only be made public after the exploitation.

Where will the data be made available?

If already known, please provide a repository per dataset or data type.

- KU Leuven RDR (Research Data Repository)
- Other data repository (specify below)

Engrxiv

When will the data be made available?

- Upon publication of research results

Which data usage licenses are you going to provide?

If none, please explain why.

- CC-BY 4.0 (data)
- MIT licence (code)

Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.

- Yes, a PID will be added upon deposit in a data repository

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

No cost foreseen except from the publication (open access) costs which will be paid by the SPROUT publication budget.

Responsibilities

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

Prof. Leblebici and Prof. Jef Vleugels.

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

Prof. Leblebici and Prof. Jef Vleugels.

Who will manage data preservation and sharing?

Prof. Leblebici and Prof. Jef Vleugels.

Who will update and implement this DMP?

Prof. Leblebici