High-tech sensors for monitoring the release of per-and polyfluoroalkyl substances (PFAS) from recycled plastic in a circular economy

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	ll)ata lvna		Data volume	Physical volume
		or E(xisting	Indicate: D(igital) or P(hysical)	Indicate: Audiovisual Images Sound Numerical Textual Model SOftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
1	Synthesis protocols for PFAS receptors	N	D	T	.docx	< 1 GB	
2	Analytical assay	N	D	T	.docx	< 1 GB	
3	Receptor-functionalized chips and wires (the chips were already designed in H2020 Remedia)	N	Р	Physical objects		NA	ca. 50 chips (25 mm by 25 mm by 1 mm) and 25 wires (5 cm long, 0.5 mm diameter)
	Images of receptor-functionalized chips and wires	N	D	I	J1 3'	< 100 GB	
5	Software for sample evaluation	E	D	SO SO	Labview	< 1 GB	
6	Data sets for sensor calibration	N	D	N, T	.txt, .xlsx	< 1 GB	
7	Presentations	N	D	A	.pptx	< 1 GB	
8	Publications and thesis	N	D	Т	.docx, .pdf	< 1 GB	

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:

The sensor chips will have the same design as those used in H2020 Remedia: this design is not yet published, but once the publication is ready and accepted, we will add the corresponding doi number to this document.

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.

No

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).

All data that are created with electronic instruments (electrochemical measurements, optical- and atomic-force microscopy) come automatically with the instrument settings as metadata. We will also preserve the instrument settings in physical- and electronic lab books and will generate an electronic read-me file that is kept is kept together with the original, measured data.

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.

No

The project is at the merge between physics, analytical chemistry, sensor development and environmental monitoring. There is no established metadata standard for such an interdisciplinary field.

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)
- Large Volume Storage

The data are stored on the laptops of the research group and on the backup servers of the Department of Physics and Astronomy.

How will the data be backed up?

• Standard back-up provided by KU Leuven ICTS for my storage solution

The backup procedures are automated and performed once daily.

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?

The data are accessible for the PI (Patrick Wagner), the Ph.D. student (Fatemeh Ahmadi Tabar), and for a second Ph.D. student (Soroush Bakhshi Sichani), who is maintaining and curating the software and electronic instruments used by Fatemeh Ahmadi Tabar. To access the data, one needs to log in to the server via the password-protected office- and measurement laptops.

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

The costs for data storage and labor of the ICT specialist are covered by the allowance (werkingsmiddelen en rekeneenheden) that the Department of Physics and Astronomy receives annually from KU Leuven. This allowance is sufficient and the research group of Patrick Wagner does not need to contribute financially.

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

The 10 years hold for all data that can be stored electronically. The sensor chips and functionalized wires will contain PFAS compounds after being used and therefore they will be disposed as chemical waste. There are no human substances involved.

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

KU Leuven RDR

KU Leuven RDR is for us the most facile option since all electronic data together will be less than 200 MB, being far below the 50 GB that KU Leuven offers per year and per researcher for free. Even all projects together that are performed by the research time will never exceed 50 GB.

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

Not applicable, we only need to preserve data for 10 years after the project since no medical data are involved.

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 restricted data (upon approval, or institutional access only)

Publications that emerge from the project will be openly available, except in cases that LIRIAS sets an embargo period. All sensor-related data (synthesis protocols for the receptors, results of electrochemical measurements, images) will be made freely available to members of the Department of Physics and Astronomy). Third parties can get access upon a motivated request, to be send to Patrick Wagner. Specifically, this holds for the promoter prof. Bart van Grinsven at Maastricht University because Fatemeh Ahmadi Tabar is going for an inter-university Ph.D. between KU Leuven and Maastricht University.

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

Research institutes outside KU Leuven can get access to the data upon sending a motivated request to Patrick Wagner, either by e-mail or with a letter. Since this project is subject to a cooperation agreement between KU Leuven and Maastricht University, we will also consult the colleagues at UMaastricht before sharing data with third parties.

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

The project is not expected to bring about new patents, but the hot-wire technique is covered by two patents owned by KU Leuven. Suppose that combining the receptors with the hot-wire transducer gives positive results (to be tested during the next months), it will be an asset in valorizing the hot-wire patents via licensing them to a company.

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)

KU Leuven RDR is our preferred option.

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)
- Data Transfer Agreement (restricted data)

Two articles coming forward from this project have been published under a CC-BY 4.0 license and two more publications are about to come. If those are not under a CC-BY 4 (depending on the journals that will accept the work), LIRIAS will set the embargo.

A data transfer agreement will be signed in all cases that are made available to third parties (institutes, companies, universities) and such agreement will be drawn up my LRD. Maastricht University can be exempted because there is already a cooperation agreement in place.

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

All publications come with a DOI number (standard practice with serious publishers).

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

Given the limited amount of data, we can share them via email or WeTransfer at no cost.

Responsibilities

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

Patrick Wagner, the technical implementation is done by Soroush Bakhshi Sichani.

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

Bert Keyaerts, senior member of the ICT staff at the Department of Physics and Astronomy.

Who will manage data preservation and sharing?

Patrick Wagner

Who will update and implement this DMP?

Patrick Wagner