FWO DMP Template - Flemish Standard Data Management Plan

Version KU Leuven

Project supervisors (from application round 2018 onwards) and fellows (from application round 2020 onwards) will, upon being awarded their project or fellowship, be invited to develop their answers to the data management related questions into a DMP. The FWO expects a **completed DMP no later than 6 months after the official start date** of the project or fellowship. The DMP should not be submitted to FWO but to the research co-ordination office of the host institute; FWO may request the DMP in a random check.

At the end of the project, the **final version of the DMP** has to be added to the final report of the project; this should be submitted to FWO by the supervisor-spokesperson through FWO's e-portal. This DMP may of course have been updated since its first version. The DMP is an element in the final evaluation of the project by the relevant expert panel. Both the DMP submitted within the first 6 months after the start date and the final DMP may use this template.

The DMP template used by the Research Foundation Flanders (FWO) corresponds with the Flemish Standard Data Management Plan. This Flemish Standard DMP was developed by the Flemish Research Data Network (FRDN) Task Force DMP which comprises representatives of all Flemish funders and research institutions. This is a standardized DMP template based on the previous FWO template that contains the core requirements for data management planning. To increase understanding and facilitate completion of the DMP, a standardized **glossary** of definitions and abbreviations is available via the following link.

	1. General Project Information
Name Grant Holder & ORCID	Xi Zhang & Orcid: 0000-0001-9519-2567
Contributor name(s) (+ ORCID) & roles	Promoter: Raf Dewil, Orcid: 0000-0003-4717-5484
	Co-promoter: Deirdre Cabooter, Orcid: 0000-0001-5502-5801
Project number 1 & title	PDMT2/23/046, Activation of periodate by transitional metal single-atom decorated biochar catalysts for
	the efficient degradation of pharmaceutically active compounds in wastewater
Funder(s) GrantID ²	KU Leuven Internal Funds: Postdoctoral mandate KU Leuven (PDM)
Affiliation(s)	☑ KU Leuven
	☐ Universiteit Antwerpen
	☐ Universiteit Gent
	☐ Universiteit Hasselt
	□ Vrije Universiteit Brussel
	□ Other:
	ROR identifier KU Leuven: 05f950310

¹ "Project number" refers to the institutional project number. This question is optional. Applicants can only provide one project number.

² Funder(s) GrantID refers to the number of the DMP at the funder(s), here one can specify multiple GrantIDs if multiple funding sources were used.

Please provide a short project description

Pharmaceutically active compounds (PhACs) are significant emerging contaminants in wastewater, posing risks to the environment and human health. Periodate(PI)-based advanced oxidation processes(AOPs) are highly promising due to PI's chemical stability during transportation and storage, and activation susceptibility. Decorating single transition metal atoms on biochar (SACs@B) combines the advantages of effective homogeneous catalytic materials with the possibility of the reuse of stabilized catalysts, representing one of the most active frontiers in catalysis. There are currently no reports on the activation of PI using such advanced SACs. There is hence an urgent need to fill this research gap. This proposal aims to design, synthesize and implement transition metal single-atom catalysts (i.e., Fe, Cu and Mn) decorated on walnut shell biochar (WSB) for the efficient catalytic activation of PI for the degradation of PhACs. First, innovative WSB and SACs@B will be synthesized and fully characterized. Second, they will be applied for the first time to activate PI to degrade PhACs. Different operating parameters will be optimized. The degradation mechanism will be evaluated through quenching experiments, ESR, XPS, kinetic modelling, and DFT calculations. Finally, Respirometry measurements will be performed to reveal the detoxification effect of treated solutions, and ECOSAR predictive models will be developed to assess the potential acute and chronic toxicity of degradation products.

2. 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 ³.

				ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR PHYSICAL DATA
Dataset	Description	New or Reused	Digital or	Digital Data Type	Digital Data	Digital Data	Physical Volume
Name			Physical		Format	Volume (MB, GB,	
						TB)	
		☐ Generate new	☐ Digital	☐ Audiovisual		□ < 1 GB	
		data	☐ Physical	☐ Images		□ < 100 GB	
		☐ Reuse existing		☐ Sound		□ < 1 TB	
		data		☐ Numerical		□ < 5 TB	
				☐ Textual		□ > 5 TB	
				☐ Model		□NA	
				☐ Software			
				☐ Other:			
Microscopy	SEM, TEM	Generate new data	Digital	Images	.tif	< 100 GB	
Images					.jpg		
					.png		
XPS, XRD,	Material	Generate new data	Digital	Images	.txt	< 100 GB	
EDX, BET, FT-	characterization			Numerical	.csv		
IR, XAFS,				Textual	.pdf		
STEM					.xlsx		
UV-VIS	Chemical	Generate new data	Digital	Numerical	.txt	10 GB	
	composition by				.xlsx		
	UV-VIS						
HPLC	Concentration	Generate new data	Digital	Images,	.dat	< 100 GB	

³ Add rows for each dataset you want to describe.

measurement	of the pollutants			Numerical,	.txt		
S				Textual	.csv		
					.xlsx		
					.pdf		
Modeling	DFT	Generate new data	Digital	Simulation	.mat / .txt /.top	< 100 GB	
data					/.JPG /.png /.gif		
Lab Notes	In notebooks,	Generate new data	Physical	-	-	-	5-10 notebook
	written details						
	about the						
	different						
	process trials,						
	results, and						
	observations						
Electronic lab	Written details	Generate new data	Digital	Images,	.txt	< 1 GB	
logbooks	about the			Textual	.xlsx		
	different				.docx		
	process trials,						
	experimental						
	conditions, and						
	observations						
Samples and	Experimental	Generate new data	Physical	-	-	-	< 10 cm ³
catalysts	samples	Reuse existing data					
Experimental	Experimental	Generate new data	Digital	Images	.tif	< 5 TB	
protocols,	results,			Numerical	.jpg		
results,	Processed and			Textual	.png		
conclusions.	analyzed			Model	.txt		
Analyzed	experimental			Origin	.dat		
papers	data				.CSV		
					.opju		
					.pdf		

Figures, datasets, drafts of research articles	Experimental results, Processed and analyzed experimental data	Generate new	data Digital	Images Numerical Textual Model Origin	.tif .jpg .png .txt	< 5 TB	
ranging from ro valuable, difficu	nw data to processed a llt to replace and/or et documentation is an in	nd analysed data hical issues are a	including analysis so ssociated. Materials	cripts and code. Physico that are not considere	al data are all mate d data in an RDM c	rials that need proper nontext include your own	ncompasses the whole spectrun management because they are n manuscripts, theses and
source, prefer	kisting data, please spably by using a persist DOI, Handle, URL etca type.	stent	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)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.		\square Yes, animal dat	oject data; provide S ta; provide ECD refer provide approval nun ation:	ence number:	al number:		
Will you process personal data ⁴ ? 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).		☐ Yes (provide PF ☐ No Additional information	RET G-number or EC	S-number below)			

⁴ See Glossary Flemish Standard Data Management Plan

Does your work have potential for commercial	⊠ Yes
valorization (e.g. tech transfer, for example spin-	□ No
offs, commercial exploitation,)?	If yes, please comment: It is possible to use it in practical water treatment technology.
If so, please comment per dataset or data type	
where appropriate.	
Do existing 3rd party agreements restrict	☐ Yes
exploitation or dissemination of the data you	⊠ No
(re)use (e.g. Material/Data transfer agreements,	If yes, please explain:
research collaboration agreements)?	
If so, please explain to what data they relate and	
what restrictions are in place.	
Are there any other legal issues, such as	☐ Yes
intellectual property rights and ownership, to be	⊠ No
managed related to the data you (re)use?	If yes, please explain:
If so, please explain to what data they relate and	
which restrictions will be asserted.	

3. Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information All collected data will be labelled for each experiment and a table with a summary for every necessary to keep data understandable and experiment will be provided. This table contains the date at which data was acquired, sample description (name/s of compound/s, concentration/s, and labelling), measurement parameters usable, for yourself and others, now and in the (Type and model of Instrument), report of results and short conclusion, suggestions towards future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab follow-up experiment. Further, a detailed description of how to prepare the samples (for both Notebooks, README.txt files, Codebook.tsv etc. successful as well as unsuccessful results) will be written and kept in Microsoft Word in KU Leuven where this information is recorded). OneDrive with regular backups. RDM guidance on documentation and metadata. All data (experimental raw data, processed data, literature review reports, and presentations related to work progress and conferences) will be stored on the KU Leuven personal drive, and can be provided to interested parties upon request. Will a metadata standard be used to make it ☐ Yes easier to find and reuse the data? \bowtie No If ves. please specify (where appropriate per dataset or data type) which metadata standard will be used: If so, please specify which metadata standard will be used. If not, please specify which metadata will be created to make the data If no, please specify (where appropriate per dataset or data type) which metadata will be created: easier to find and reuse. REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.

4. Data Storage & Back-up during the Research Project

Where will the data be stored?	☐ Shared network drive (J-drive)
	☐ Personal network drive (I-drive)
Consult the interactive KU Leuven storage guide to	☐ OneDrive (KU Leuven)
find the most suitable storage solution for your data.	☐ Sharepoint online
	☐ Sharepoint on-premis
	☐ Large Volume Storage
	☐ Digital Vault
	☑ Other: 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.
How will the data be backed up?	☐ Standard back-up provided by KU Leuven ICTS for my storage solution
•	□ Personal back-ups I make (specify):
WHAT STORAGE AND BACKUP PROCEDURES WILL BE IN PLACE TO PREVENT DATA LOSS?	The data will be backed-up automatically for remote data storage on a daily basis in the cloud using KU Leuven one-drive storage and kept on the measurement equipment/PC where possible. Additionally, other copies of the data will be kept at different physical locations using portable hard drives. Physical samples are stored in sample boxes in the lab/departmental storage room. □ Other (specify)
Is there currently sufficient storage & backup	⊠ Yes
capacity during the project? If yes, specify	□ No
concisely. If no or insufficient storage or backup	
capacities are available, then explain how this	If no, please specify:
will be taken care of.	

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons? CLEARLY DESCRIBE THE MEASURES (IN TERMS OF PHYSICAL SECURITY, NETWORK SECURITY, AND SECURITY OF COMPUTER SYSTEMS AND FILES) THAT WILL BE TAKEN TO ENSURE THAT STORED AND TRANSFERRED DATA ARE SAFE. Guidance on security for research data	Both during and after the project, data will be stored using the KU Leuven central network drives (as an automatic back-up), and on the OneDrive storage provided by KU Leuven. On KU Leuven personal drive there are strict authorizations in place so no external/unauthorized user can access the data. Each KU Leuven-associated PC requires username and password, which must be changed every year.
What are the expected costs for data storage and backup during the research project? How will these costs be covered?	Using KU Leuven's OneDrive to store data does not require additional payment. I also have a personal hard drive that can be used to store data without paying extra.

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...). 5. Data Preservation after the end of the Research Project All data will be preserved for 10 years according to KU Leuven RDM policy All data will be preserved for 25 years according to CTC recommendations for clinical trials with medicinal products for human use and for clinical experiments on humans Certain data cannot be kept for 10 years (explain) Guidance on data preservation

Where will these data be archived (stored and	⊠ KU Leuven RDR
curated for the long-term)?	☐ Large Volume Storage (longterm for large volumes)
	☐ Shared network drive (J-drive)
<u>Dedicated data repositories</u> are often the best place	☑ Other (specifiy): KU Leuven Onedrive
to preserve your data. Data not suitable for	
preservation in a repository can be stored using a KU	
Leuven storage solution, consult the interactive KU	
<u>Leuven storage guide</u> .	
What are the expected costs for data	Using KU Leuven's onedrive to store data does not require additional payment. I also have a personal hard
preservation during the expected retention	drive that could also be used to store data without paying extra.
period? How will these costs be covered?	

6. Data Sharing and Reuse				
Will the data (or part of the data) be made available for reuse after/during the project?	☐ Yes, as open data ☐ Yes, as embargoed data (temporary restriction)			
Please explain per dataset or data type which data will be made available.	 ⊠ Yes, as restricted data (upon approval, or institutional access only) □ No (closed access) □ Other, please specify:			
NOTE THAT 'AVAILABLE' DOES NOT NECESSARILY MEAN THAT THE DATA SET BECOMES OPENLY AVAILABLE, CONDITIONS FOR ACCESS	Other, please specify.			
AND USE MAY APPLY. AVAILABILITY IN THIS QUESTION THUS ENTAILS BOTH OPEN & RESTRICTED ACCESS. FOR MORE INFORMATION: HTTPS://WIKI.SURFNET.NL/DISPLAY/STANDARDS/INFO-EU-REPO/#INF OEUREPO-ACCESSRIGHTS				

All relevant data and findings will be published in peer-reviewed journals that can be accessed online by
anyone with access to the relevant website.
These publications will also be stored on KU Leuven's Lirias platform and can be accessed by colleagues
and students at KU Leuven.
e ☐ Yes, privacy aspects
☐ Yes, intellectual property rights
☐ Yes, ethical aspects
☐ Yes, aspects of dual use
☐ Yes, other
⊠ No
If yes, please specify:
⊠ KU Leuven RDR
☐ Other data repository (specify)
☐ Other (specify)
□ Upon publication of research results
☐ Specific date (specify)
☐ Other (specify)

Which data usage licenses are you going to provide? If none, please explain why. A DATA USAGE LICENSE INDICATES WHETHER THE DATA CAN BE REUSED OR NOT AND UNDER WHAT CONDITIONS. IF NO LICENCE IS GRANTED, THE DATA ARE IN A GREY ZONE AND CANNOT BE LEGALLY REUSED. DO NOTE THAT YOU MAY ONLY RELEASE DATA UNDER A LICENCE CHOSEN BY YOURSELF IF IT DOES NOT ALREADY FALL UNDER ANOTHER LICENCE THAT MIGHT PROHIBIT THAT. Check the RDR quidance on licences for data and software sources code or consult the License selector tool to help you choose.	 □ CC-BY 4.0 (data) □ Data Transfer Agreement (restricted data) □ MIT licence (code) □ GNU GPL-3.0 (code) □ Other (specify)
Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, please provide it here. INDICATE WHETHER YOU INTEND TO ADD A PERSISTENT AND UNIQUE IDENTIFIER IN ORDER TO IDENTIFY AND RETRIEVE THE DATA. What are the expected costs for data sharing? How will these costs be covered?	 ✓ Yes, a PID will be added upon deposit in a data repository ☐ My dataset already has a PID ☐ No Using KU Leuven's OneDrive to share data does not require additional payment. I also have a personal hard drive that could also be used to share data without paying extra.

	7. Responsibilities
Who will manage data documentation and	Xi Zhang
metadata during the research project?	
Who will manage data storage and backup	Xi Zhang
during the research project?	
Who will manage data preservation and	Xi Zhang
sharing?	
Who will update and implement this DMP?	Xi Zhang