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	**Xing Yang 0000-0002-8403-8254**
Contributor name(s) (+ ORCID) & roles	**Giuseppe Granata 0000-0001-6593-6270**
Project number [1] & title	**inteGRating mEchnochEmistry aNd mEmbranes for lithium-ion battery Recycling: a closed-loop route (GREENER)**
Funder(s) GrantID [2]	
Affiliation(s)	X KU Leuven ☐ Universiteit Antwerpen ☐ Universiteit Gent ☐ Universiteit Hasselt ☐ Vrije Universiteit Brussel ☐ Other: ROR identifier KU Leuven: 05f950310

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[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	Aiming to address the current challenges in Li-ion battery (LIB) recycling associated with the low recovery rate and low purity of recycled materials, the GREENER project proposes a new technical route that integrates novel mechanochemical processing (MP) and membrane technology (MT) to produce industry-grade materials readily available for cathode re-synthesis. A novel MP method will be investigated to increase the yield and selectivity in Li extraction from LIBs waste and achieve the separation of Ni, Mn and Co (obj.1). An integrated process of selective electrodialysis and membrane crystallization with tailored membranes/units will be designed to purify the metal-rich solutions produced by MP, with the aim to identify process controlling parameters for maximal recovery of battery-grade hydroxides of Li, Ni, Mn and Co (obj.2). A MP-assisted method will be developed to resynthesize NMC811 cathodes from the purified battery-material streams (Obj. 3). The performance of the as-obtained NMC811 as cathodes for LIBs will finally be demonstrated. Such integration route has never been explored in the field, hence will be a new contribution to both scientific community and industrial process development. The proposed multidisciplinary approach will impact theories and applications of separation technologies in the domain of sustainable energy.

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 Name	Description	New or Reused	Digital or Physical	Digital Data Type	Digital Data Format	Digital Data Volume (MB, GB, TB)	Physical Volume
		☐ Generate new data ☐ Reuse existing data	☐ Digital ☐ Physical	☐ Audiovisual ☐ Images ☐ Sound ☐ Numerical ☐ Textual ☒ Model ☐ Software ☐ Other:		☐ < 1 GB ☐ < 100 GB ☐ < 1 TB ☐ < 5 TB ☐ > 5 TB ☐ NA	
Lab notes	Description of the practical execution of experiments	New	Digital and if Physical, they will be digitalized as materials and method section	Observational and experimental	NA	NA	5-10 note books
Filtration results	Conditions &	New	Digital	Experimental	.xlsx	< 1 GB	

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[3] Add rows for each dataset you want to describe.

	Results form the filtration experiments						
Mechanochemical milling experiments	Conditions & results of Mechanochemical milling experiments	New	Digital	Experimental	.xlsx	< 1 GB	
Infrared radiation (IR)	infrared spectroscopy data	New	Digital	Experimental	.xlsx/.dpt/.0	< 1 GB	
Density measurements	Density measurement data	New	Digital	Experimental	.xlsx	< 100MB	
Ion transport/ adsorption experiments	Ion transport/ adsorption experiment data	New	Digital	Experimental	.xlsx	< 1 GB	
Structural characterization	Structure of materials, e.g., XRD	New	Digital	Experimental	.raw, .dif	< 1 GB	
Electrochemical measurements	Electrochemical workstation data	New	Digital	Experimental	.xlsx	< 1 GB	
Microscopy data	SEM, TEM, AFM	New	Digital	Experimental	.CVS, pdf, .tif	< 10 GB	
Elemental mapping	SEM-EDS / XPS	New	Digital	Experimental	.xlsx	< 10 GB	

Thermal measurements	Thermal analysis of materials, e.g., TG-DTA	New	Digital	Experimental	.xlsx	< 1 GB	
Solution property characterization	Quantification of solution properties such as ion concentration using ICP-OES	New	Digital	Experimental	.xlsx	< 1 GB	
Particle property measurements	Particle properties, e.g., size, PSD using master sizer	New	Digital	Experimental	.xlsx	< 1 GB	
Thermodynamic modeling	Results of thermodynamic modeling, e.g., HSC Chemistry calculation.	New	Digital	Modeling	.HSC	< 1 GB	
Fluid dynamic modeling	Results of fluid dynamic modeling, e.g., CFD simulations, MATLAB	New	Digital	Modeling	.m, .docx, .xlsx .MPH	< 1 TB	

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.	NA
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.	☐ Yes, human subject data; provide SMEC or EC approval number: ☐ Yes, animal data; provide ECD reference number: ☐ Yes, dual use; provide approval number: ☒ No Additional information:
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 PRET G-number or EC S-number below) ☒ No Additional information:
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 ☒ No If yes, please comment:

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[4] See Glossary Flemish Standard Data Management Plan

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 to what data they relate and what restrictions are in place.	☒ Yes ☐ No If yes, please explain: The use of commercial monovalent ion exchange membranes will require a MTA that has already existed between the supplier (i.e., Eurodia) and KU Leuven.
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 to what data they relate and which restrictions will be asserted.	☒ Yes ☐ No If yes, please explain: Regarding the MTA with Eurodia, there is certain restriction on the chemical composition of the membrane materials, where the supplier provided certain manufacturing data. There is no restriction on the results obtained from testing/performance of the materials.

3. 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).
 	
RDM guidance on documentation and metadata.
	The approach to capture the accompany information necessary to keep data understandable and usable is dependent on the types of data:
	    1. **Data related to experimental design, testing conditions/settings and raw data, for example,**
	Notes: The electronic lab notebook is used for setup design (sketches) and writing down of observations. This notebook will be stored in KU Leuven drives.
	Manuscripts: Communication of scientific results is done via manuscripts and saved in .docx, .pdf or .tex.
	Presentations: Presentations containing scientific results are produced using PowerPoint and stored accordingly (.ppt or .pdf).
	
	    2. **Data related to analytical measurements, for example,**
	Solution property measurements, e.g., ICP-OES: Samples are prepared according to SOPs and named "name_D/C_time". Observations and procedures are reported in a handwritten lab book and subsequently noted digitally (.docx, .xlsx). Data are received in .csv and .xlsx format.
	Microscopy Images: Pictures are taken according to SOPs, saved in .tiff and named "name_type_conditions", as the device settings are displayed on the pictures taken. ImageJ software can be used to analyze the images and produce particle size distributions with the use of MATLAB or origin software.
	Material elemental and structural measurements, e.g, Infrared Spectroscopy, XRD, etc: Samples are prepared according to SOPs and named "name_type_conditions". Observations and procedures are digitally reported in a lab notebook.
	After operation, physical liquid/solid samples are not stored but some imaging samples can be partially recuperated.
	    3. **Data related to modelling or theoretical calculations, for example,**
	These CFD models will be constructed using COMSOL software. For each model, multiple simulations files of .mph format will be generated with labelling ("WPnumber_modelname_conditions"). Moreover, .docx file will be made to accompany each model file and will contain all the simulation conditions and observations and .xlsx files for output plots and graphs.
	MATLAB Codes: These codes will be constructed using MATLAB software. For each workpackage that requires coding, different script files of .m format will be generated with labelling ("WPnumber_modelname_correlationtype"). Moreover, .docx file will be made to accompany each code

	file and will contain all the simulation conditions and observations and .xlsx files for output plots and graphs. Thermodynamic simulations: These codes will be constructed using HSC Chemistry software. For each model, multiple simulations files of .HSC format will be generated with labelling ("WPnumber_modelname_conditions"). Moreover, .docx file will be made to accompany each model file and will contain all the simulation conditions and observations and .xlsx files for output plots and graphs.
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. *REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.*	☐ Yes ☒ No If yes, please specify (where appropriate per dataset or data type) which metadata standard will be used: If no, please specify (where appropriate per dataset or data type) which metadata will be created:

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

Where will the data be stored? *Consult the [interactive KU Leuven storage guide](#) to find the most suitable storage solution for your data.*	☐ Shared network drive (J-drive) ☐ Personal network drive (I-drive) ☒ OneDrive (KU Leuven) ☒ Sharepoint online ☐ Sharepoint on-premis ☐ Large Volume Storage ☐ Digital Vault ☐ Other:

How will the data be backed up? *WHAT STORAGE AND BACKUP PROCEDURES WILL BE IN PLACE TO PREVENT DATA LOSS?*	☐ Standard back-up provided by KU Leuven ICTS for my storage solution ☒ Personal back-ups I make (specify) ☐ Other (specify) Data are backed up on the cloud (OneDrive) immediately. The software indicates the update status (green, blue or red) and, in case of a nonsync, action can be taken using the online version of the tool. Data are further back up regularly on an external hard drive. After completion of (sub)WPs, data will be additionally backed up on the KUL service servers.
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 ☐ No Maximum data storage should not exceed 2 TB per project If no, please specify:
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*	The accesses to OneDrive and SharePoint are only for researchers with permission. All users need to use a two-factor Authenticator (2FA app used at KUL). Furthermore, a log-out is always performed when leaving Lab PCs (where data is generated) to prevent modification of parameters by unauthorized people.
What are the expected costs for data storage and backup during the research project? How will these costs be covered?	The estimated costs for data storage and back up during the project will not exceed 5000€. These costs will be covered and shared by both PIs of the project.

5. 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...). _Guidance on data preservation_	☐ 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) All the data will be retained for the expected 5 years period after the end of the project with no exceptions.
Where will these data be archived (stored and curated for the long-term)? _Dedicated data repositories are often the best place 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 Leuven storage guide._	☒ KU Leuven RDR ☐ Large Volume Storage (longterm for large volumes) ☐ Shared network drive (J-drive) ☐ Other (specifiy): All the data will be stored for the long-term on the KUL service servers (with automatic back-up procedures), conforming with KUL RDM policy.
What are the expected costs for data preservation during the expected retention period? How will these costs be covered?	The estimated costs for data storage and archiving after the project will be around 5000€. These costs will be covered and shared by both PIs of the project.

6. 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. *NOTE THAT 'AVAILABLE' DOES NOT NECESSARILY MEAN THAT THE DATA SET BECOMES OPENLY AVAILABLE, CONDITIONS FOR ACCESS 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/#INFOEUREPO-ACCESSRIGHTS*	☒ Yes, as open data ☒ Yes, as embargoed data (temporary restriction) ☒ Yes, as restricted data (upon approval, or institutional access only) ☐ No (closed access) ☐ Other, please specify: Data relevant for publication will be made available in an Open Access repository (i.e.,Lirias). Full datasets will only be made available upon request.
If access is restricted, please specify who will be able to access the data and under what conditions.	NA
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, privacy aspects ☒ Yes, intellectual property rights ☐ Yes, ethical aspects ☐ Yes, aspects of dual use ☐ Yes, other ☐ No If yes, please specify: If there is any patentable results or patents, the IP rights will be reserved. For example, new methods for mechanochemical treatment, or new processes developed for ion fractionation.
Where will the data be made available? If already known, please provide a repository per dataset or data type.	☒ KU Leuven RDR ☐ Other data repository (specify) ☐ Other (specify)

When will the data be made available?	☒ 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 guidance 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) This is mainly applicable to data generated by non-open source software, for example, for CFD models, COMSOL license will be provides with the appropriate modules. For MATLAB Codes: MATLAB License will be provided
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.*	☐ Yes, a PID will be added upon deposit in a data repository ☐ My dataset already has a PID ☒ No
What are the expected costs for data sharing? How will these costs be covered?	The expected cost for data sharing is 0€. Free tools like Belnet FileSender (KUL account) will be used for data sharing. In the unlikely event that there would be costs, these costs will be covered by project budget, or both PIs of the project.

7. Responsibilities	
Who will manage data documentation and metadata during the research project?	Prof. Xing Yang Prof. Giuseppe Granata

Who will manage data storage and backup during the research project?	Prof. Xing Yang Prof. Giuseppe Granata
Who will manage data preservation and sharing?	Prof. Xing Yang Prof. Giuseppe Granata
Who will update and implement this DMP?	Prof. Xing Yang and Prof. Giuseppe Granata bear the end responsibility of updating and implementing this DMP in the long term.