
INTRODUCING POROUS ORGANIC MOLECULES INTO ADVANCED MEMBRANE FOR LITHIUM EXTRACTION

A Data Management Plan created using DMPonline.be

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Template: FWO DMP (Flemish Standard DMP)

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Project abstract:

It is predicted that the continuously increasing demand for the energy-critical element of lithium will soon exceed its availability, rendering it a geopolitically significant resource. Lithium (Li⁺) extraction from salt lake brines is an effective way to circumvent the lithium supply shortage. Given the close hydrated radius of Mg²⁺ (4.3 Å) and Li⁺ (3.8 Å) ions, a facile membrane synthesis method is needed to fabricate membranes for efficient Li extraction from high Mg²⁺/Li⁺ ratio brines. Porous organic molecules (POMs) with inner cavity diameter from 3.2 to 4.3 Å, such as cyclodextrin, calixarene, cucurbituril, and pillararene, will be used as main building blocks to construct NF membranes with uniform sub-nanometer pores for precise ion-ion separation. Furthermore, the fundamental mechanisms underlying cations transport and selectivity in subnanometer pores will be elucidated to provide the scientific base for the design of NF membranes with high Li⁺ selectivity.

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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
Dataset Name	Description	New or reused	Digital or Physical	Digital Data Type	Digital Data format	Digital data volume (MB/GB/TB)	Physical volume
		<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Generate new data Reuse existing data 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Digital Physical 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Observational Experimental Compiled/aggregated data Simulation data Software Other NA 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> .por, .xml, .tab, .cvs, .pdf, .txt, .rtf, .dwg, .gml, ... NA 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <100MB <1GB <100GB <1TB <5TB <10TB <50TB >50TB NA 	
Selection of POMs	The monomer pore size information and chemical properties will be summarised and screened, and Excel data will be generated	New data	Digital	Experimental	.xlsx	<100MB	
Functional POMs	POMs monomers will be modified and functionalized according to separation characteristics,	New data	Digital	Experimental	.xlsx	<100MB	
Fabrication NF membranes	NF membranes with high permeability and Li+ extraction will be prepared	New data	Digital	Experimental	.xlsx	<100MB	
NF filtration text	The determination of the actual separation of high Mg2+/Li+ ratio brines solution	New data	Digital	Experimental	.xlsx	<100MB	
NF membrane characterisation	SEM, AFM, TEM, XPS, Zeta, FTIR, WCA	New data	Digital	Experimental	.pdf	<1GB	
Fundamental mechanisms of ion transport	An electric field as a driving force will be used to decouple the transport of cations through the sub-nanometer pores to determine the energy barriers for the permeation of cations	New data	Digital	Experimental Simulation data	.xlsx	<100MB	
Fundamental mechanisms of ion selectivity	A density functional theory simulation will be performed to explore the influence of the electrostatic interactions between the permeating ions and the fixed charge on the membrane.	New data	Digital	Experimental Simulation data	.xlsx	<100MB	

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:

No

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.

- Yes

The project may lead to a novel nano filtration membrane, for which IP rights may be acquired in the future.

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).

Each dataset will be stored in a separate folder in my KU Leuven Onedrive. The name of each document will contain only contain the information relevant to its content.

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.

- Yes

I will use the metadata standard of KU Leuven Research Data Repository.

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

Where will the data be stored?

KU Leuven Onedrive and a personal hard drive.

How will the data be backed up?

The KU Leuven Onedrive frequently makes a back-up. Furthermore, I will regularly update the storage on my personal hard drive.

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

KU Leuven one drive provides 2000 GB storage. This far exceeds the expected storage needed for my research.

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

The personal KU Leuven Onedrive can only be accessed by the personal institutional login.

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

NA

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 datasets previously described.

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

KU Leuven Onedrive.

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

NA

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.

- Yes, in a restricted access repository (after approval, institutional access only, ...)

Only published data will be available in the form of publications or other dissemination of scientific work. All data will be anonymised when disseminated. More data can be made available or shared after permission of the responsible person (PENGRUI JIN). Non-published data will remain confidential until a final decision on publication of the data has been taken.

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

Data could be reused by other members of the BVDB team, after consultation and approval of the head of our lab group and/or the head of BVDB team (prof. Bart Van der Bruggen).

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.

A specific repository will be chosen after the publication strategy is known as some journal request specific repositories.

When will the data be made available?

Only after publication of the research results in a peer-reviewed journal.

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

Collected data: For meta-analytic projects researchers can request the full pseudonymized dataset via email, and will receive these after signing a data-sharing agreement. For published papers, a trimmed and pseudonymized dataset (i.e., only containing the variables required to reproduce our results) will be uploaded in a .csv or .xlsx format to the Open Science Framework under a CC-BY license alongside full dataset documentation. Participants' personal information (e.g., contact information, names, etc.) will never be shared

Simulated data: Simulated data will be made available upon request by other researchers. Codes will be uploaded to the Open Science Framework and/or Github.

Software: the R-package and associated functions will be uploaded on CRAN and Github under a GPL license.

Do you intend to add a PID/DOL/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- Yes

Depending on the data repository and the type of data that would be made available, a unique identifier will be added to the data set.

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

NA

6. Responsibilities

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

PENGRUI JIN, BART VAN DER BRUGGEN

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

PENGRUI JIN, BART VAN DER BRUGGEN

Who will manage data preservation and sharing?

PENGRUI JIN, BART VAN DER BRUGGEN

Who will update and implement this DMP?

PENGRUI JIN, BART VAN DER BRUGGEN