
NMR-Relaxorption: Measuring and understanding NMR relaxation during sorption in porous materials

A Data Management Plan created using DMPonline.be

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Funder: KU Leuven (KUL)

Template: KU Leuven BOF-IOF

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Grant number / URL: C14/21079

ID: 200590

Start date: 01-10-2021

End date: 30-09-2025

Project abstract:

Porosimetry is an important and recurrent analysis in material chemistry characterization. Materials such as metal-organic frameworks (MOFs), mesoporous silicas, and zeolites are typically characterized using gas/vapor adsorption and desorption isotherms. Through the controlled partial pressure loading of an evacuated sample volume, this technique determines indirectly qualitative and quantitative properties of the pore environment, like BET surface area and pore volume, with limited insight into the quantifiable nature of guest/host interactions. Low-field Nuclear Magnetic Resonance (LF-NMR) Relaxometry is applied commonly to porous media analysis to directly measure the content and physicochemical properties of the porous environment through nuclear spin relaxation of the contained liquid. In this project, we combine both techniques to obtain complementary information in situ, in operando. Time resolved relaxation analysis will inform us about the dynamics of the guest molecules and the interactions with the pore walls as a function of loading throughout the isotherm curves. Additional information will be acquired using advanced 2DNMR methodology where correlations between relaxation times and diffusion coefficient will be demonstrated. Results will be compared with simulation data from models and for unique insight will be acquired about the sorption mechanisms in various porous materials. The outcome of the project will be a new characterization modality.

Last modified: 23-06-2023

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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 S oftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
NMR Data	Spectra from the NMR Console	N	D	SO	.tnt	<100GB	Hard disk Drive
Physisorption Data	Isotherm curves from the Sorption Analyser	N	D	SO	?	<100GB	Hard disk Drive

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:

URL

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).

The data will be stored in raw format and the associated descriptions will be listed in a word file document in order to allow understanding, reproduction if needed and exploitation in the future, if needed.

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

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)

How will the data be backed up?

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

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 the members of the project will have access to the data from the project.

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

Eject will cover these costs, which are expected to be minimal.

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)?

- KU Leuven RDR

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

These costs will be covered by the Sakellariou Lab funds, if needed.

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.

- No (closed access)

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

Only the members of the Sakellariou Lab will be able to access data, once authorisation by the PI is given.

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.

- No

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)

When will the data be made available?

- Other (specify below)

Which data usage licenses are you going to provide?

If none, please explain why.

- Data Transfer Agreement (restricted data)

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.

- No

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

We do not know if there will be costs associated with sharing the data.

Responsibilities

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

Dimitrios Sakellariou

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

Rodrigo de Oliveira Silva

Who will manage data preservation and sharing?

Rodrigo de Oliveira Silva

Who will update and implement this DMP?

Dimitrios Sakellariou

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