BESPOKE SOLID-STATE NMR PROBE-HEADS FOR NOVEL IN-SITU CHARACTERIZATION OF OPTOELECTRONIC METAL HALIDE PEROVSKITES

A Data Management Plan created using DMPonline.be

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Project abstract:

Metal halide perovskites (MHPs) display excellent optoelectronic properties providing low fabrication cost, and high-efficiency, alternative materials for photovoltaic and light emitting devices. The main obstacle to wide-spread commercial adoption is their low stability under moderate heat, moisture and even light. To improve their stability, new MHP configurations are reported frequently utilising cation mixtures, metal dopants, surface passivators, different dimensional frameworks/phases, and more. However, the key to better material design is detailed structural characterisation, which is often lacking in the rush for the highest efficiency materials. Solid-state nuclear magnetic resonance (NMR) is a proven tool for examining MHP materials at the local atomic level. This project aims to develop bespoke NMR hardware, designed specifically for the in-situ study of MHPs. Namely, magic angle spinning (MAS) NMR under irradiation to study the evolution of the MHP structure under visible light; and sensitivity-optimised MAS NMR of MHP thin films printed on slides, allowing nondestructive examination of the materials in their device format. These novel techniques will provide insight into the structure-function relationships of MHP materials in their operating conditions, revealing the degradation pathways that hinder their stability, providing a route towards state-of-the art optoelectronic devices.

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DPIA

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Have you performed a DPIA for the personal data processing activities for this project?

- Not applicable

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GDPR

GDPR

Have you registered personal data processing activities for this project?

- Not applicable

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Application DMP

Questionnaire

Describe the datatypes (surveys, sequences, manuscripts, objects …) the research will collect and/or generate and /or (re)use. (use up to 700 characters)

Expectation that all data will be generated during the project. No personal or sensitive data.
Characterisation and computational techniques raw data: nuclear magnetic resonance data stored as software specific files, majority will be Topspin. Where possible, will be stored as .txt or .csv files for accesibility.
Data analytics and graphing will be processed via excel, scidavis or origin pro and hence saved as .xlsx, .sciprj or . pju.
Notes, reports and manuscripts will be stored as .docx, .ppt or .pdf.
Diagrams and images will be stored as .png, .tiff, .svg, etc.

Specify in which way the following provisions are in place in order to preserve the data during and at least 5 years after the end of the research? Motivate your answer. (use up to 700 characters)

1. Designation of responsible person: Prof Dimitrios Sakellariou (KU Leuven)
2. Storage capacity/repository
    - during the research: KU Leuven network drives (staff personal drive 50GB; large volume data drive 1TB; Onedrive backup: 2TB
    - after the research: The KU Leuven research data management policy stipulates that relevant data generated are retained for a period of minimally 10 years after the end of the project. The same storage options are available as during the project.

What's the reason why you wish to deviate from the principle of preservation of data and of the minimum preservation term of 5 years? (max. 700 characters)

N.A.

Are there issues concerning research data indicated in the ethics questionnaire of this application form? Which specific security measures do those data require? (use up to 700 characters)

N.A.

Which other issues related to the data management are relevant to mention? (use up to 700 characters)

N.A.

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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
		Please choose from the following options: • Generate new data • Reuse existing data	*Please choose from the following options:* • Digital • Physical	*Please choose from the following options:* • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA	*Please choose from the following options:* • .por, .xml, .tab, .csv,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
Topspin raw data	NMR data	New	Digital	Experimental	Topspin data files	<100GB	
Other raw data	Other characterisation techniques: XRD, TEM, PL, XPS, etc	New	Digital	Experimental	.csv, .txt, .png	<100GB	
Data analytics	Analysis, graphing, simulation	New	Digital	Compiled/aggregated data	.xlsx, .sciprj	<1GB	
Reports	Reports, manuscipts	New	Digital	Other	.docx, .pdf., .ppt	<1GB	
Diagrams	Images	New	Digital	Other	.png, .tiff, .svg	<100GB	

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:

N.A.

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

Manufacture probeheads could be valorised. All data describing and demonstrating probeheads would be related to valorisation.

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).

README.txt files stored alongside all data.

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.

- No

Metadata produced via individual software used to create raw data.

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

Where will the data be stored?

KU Leuven network drives (staff personal drive 50GB; large volume data drive 1TB

How will the data be backed up?

Onedrive backup: 2TB

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

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

Security provided via KU Leuven network drive infrastructure.
Network laptop, stored in locked office.

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

Free

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...).

Retained for 10 years according to KU Leuven RDM policy.

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

Same as during research. Transferred to Prof Dimitrios Sakellariou if Thomas Hooper leaves KU Leuven.

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

Free

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, …)

Experimental data will be accessible after publication except in the case of valorisation.

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

Experimental data will be accessible after publication except in the case of valorisation.

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.

KU Leuven RDR

When will the data be made available?

After publication.

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

Standard terms and conditions.

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

- Yes

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

Free

6. Responsibilities

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

Thomas Hooper

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

Thomas Hooper

Who will manage data preservation and sharing?

Thomas Hooper

Who will update and implement this DMP?

Thomas Hooper