CELSA project: Single crystal PErovskite Charge Transport Engineering for high-performance Radiation detection (SPECTER)

A Data Management Plan created using DMPonline.be

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Template: KU Leuven BOF-IOF

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Project abstract:

Metal halide perovskite (MHP) semiconductors have emerged as a highly promising material class for application in the fields of photovoltaics, LEDs, and more particularly, high-energy radiation detectors. Besides their low cost and easy processing, the popularity of MHPs arises from their outstanding optoelectronic properties, such as strong high-energy radiation absorption, and efficient charge carrier generation and transport, outperforming current market standards. However, the intrinsic instability and toxicity of popular lead-based MHPs hinders their large-scale application in sustainable detector technology. The ultimate goal of SPECTER is to rationally develop Pb-free MHPs through compositional and dimensionality engineering, and perform their in-depth characterization towards application as photoactive media in next-generation high-energy radiation detectors. These will facilitate low-dose medical imaging, security and transport screening, and high- energy physics research. High-quality Pb-free MHP single crystals will be prepared, followed by carefully selected metal contact deposition. The (opto-)electric properties of the materials will be explored by a full arsenal of both established and unique characterization techniques, enabled by the complementary tool set of both SPECTER partners. Additionally, stability tests will be performed at versatile conditions: biasing, elevated temperature, humidity, long-term high-energy irradiation. The obtained functionalities will be critically analyzed and the intrinsic strengths and limitations of the material will be assessed. A fundamental understanding of the intrinsic relationships between the chemical composition, structure, charge carrier transport, defects, and material stability, will steer successive feedback loops of MHP crystal growth & characterization (4 to 6 iterations between KUL and CU expected), in order to rationally improve detector stability and performance.

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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
Perovskite single crystals	Synthesized perovskite single crystals	***N** and **E***	**P**	Physical (in)organic crystals	NA	NA	Small vials
Raw data	Raw data resulting from: e.g. spectroscopic studies, XRD measurements, ...	***N***	**D**	**I**mages **N**umerical **T**extual **M**odel	.png, .cif, .txt, .csv	<1TB	NA
Protocols	Protocols used for the realization of setups/materials	***N***	**D**	**I**mages **N**umerical **T**extual	.png, .txt	<1GB	NA
Codes for data processing	Codes used for analysis of results (data processing)	***N***	**D**	**N**umerical **T**extuall **SO**ftware	.opj, .csv, .mat	<500GB	NA
Reporting	Manuscripts and/or dissemination texts	***N***	**D**	**I**mages **T**extual	.doc, .pdf	<1GB	NA

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.

- 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).

(Electronic) Lab Notebooks
text files (.doc, .txt, .pdf)

Will a metadata standard be used to make it easier tofind 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?

- Sharepoint online
- Large Volume Storage
- 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?

No issues are expected.
Nonetheless, all data stored in the mixed MS-SP/LVS system of Debroye group are protected by the identity services of KU Leuven. This allows GxP compliant and fully traceable control over data access rights, registration of data access events and will ensure availability and safety of data well beyond the 5 year limit as these services are an integral part of KU Leuven ICT infrastructure.

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

No to negligible costs, which can be covered via personal KU Leuven seed fund.

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)?

- Large Volume Storage (longterm for large volumes)

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

No to negligible costs, which can be covered via personal KU Leuven seed fund.

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.

- Yes, as restricted data (upon approval, or institutional access only)

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

Access by both PIs, fellows appointed to the project, project supervisor.

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)

Candidate repositories will be selected throughout the course of the project.

When will the data be made available?

- Upon publication of research results

Which data usage licenses are you going to provide?

If none, please explain why.

- Other (specify below)
- CC-BY 4.0 (data)

Creative Commons Attribution-NonCommercial (CC-BY-NC)
A creative commons license that bans commercial use.

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.

- Yes, a PID will be added upon deposit in a data repository

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

Publications costs will be covered by the required budget as indicated in the CELSA proposal.

Responsibilities

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

Both PIs, fellows appointed to the project.

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

Both PIs, assisted by Dr. Haifeng Yuan who manages data storage, annotation and sharing. He collaborates with the KUL ICTS administration to maintain a data management system.

Who will manage data preservation and sharing?

Both PIs, assisted by Dr. Haifeng Yuan who manages data storage, annotation and sharing. He collaborates with the KUL ICTS administration to maintain a data management system.

Who will update and implement this DMP?

Myself, as main PI, with guidance of Dr. Haifeng Yuan and eventual KU Leuven administrators.