Plan Overview

A Data Management Plan created using DMPonline.be

Title: HP3: High-Performance Halide Perovskites through HeteroePitaxial functionalization with chalcogenides

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Funder: KU Leuven (KUL)

Template: KU Leuven BOF-IOF

Project abstract:

HP3 develops a novel approach to inhibit the degradation caused by ionic migration in Lead halide perovskite (LHP) devices. Current techniques focus on increasing activation energy or employing interlayers to limit migration. However, both strategies have their limitations. HP3 proposes a multi-pronged approach to improve LHP device performance. This approach is based on a heteroepitaxial thin film structure that combines LHPs and lead-based chalcogenides. These chalcogenides have excellent ambient stability, optoelectronic properties, thermal conductivity, and carrier mobility. HP3 will use a thick epitaxial layer of chalcogenides to provide ambient stability to LHP devices and prevent migrating halide atoms from reacting with other transport layers and electrodes. The chalcogenide epitaxial layer also offers several other benefits, including strain engineering, ambient stability, and efficient carrier transport and extraction. The HP3 aims to improve the stability and performance of LHP devices and make them more appealing for future applications.

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HP3: High-Performance Halide Perovskites through HeteroePitaxial functionalization with chalcogenides

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 **SO**ftware **O**ther (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
WP1:Single Crystal Growth Data, Heteroepitaxial Layer Deposition Data	Data related to the growth conditions, parameters, and outcomes of CsPbX3 (X = Cl, Br, I) single crystals. Data on the deposition process of chalcogenide layers on halide perovskite single crystals, including reaction conditions and outcomes.	N	D	I, N	JPEG, TIFF	<100GB	0
WP2: Structural Characterization Data and Optoelectronic Characterization Data	Data from structural characterization techniques such as XRD, GIWAXS, and TEM, used to analyze the heteroepitaxial structures. Data from optoelectronic characterization techniques including steady-state and time-resolved absorption and photoluminescence spectroscopies.	N	D	I,N	CSV, JPEG, TIFF, TXT	<100GB	0
WP3: Device Performance Data	Data on the performance of photovoltaic and self-powered photodetector devices fabricated using the heteroepitaxial structures.	N	D	I,N	CSV, JPEG, TIFF, TXT	<100GB	0

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:

I do not plan to reuse existing data.

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.

- Yes

The research has potential for commercial valorization, particularly in the development of stable and high-performance lead halide perovskite (LHP) devices. Specific datasets and their potential applications include:

1. Material Synthesis Data: Innovations in heteroepitaxial integration could lead to improved manufacturing techniques for LHP materials, benefiting industries focused on photovoltaics and optoelectronic devices.
2. Device Performance Data: Metrics such as power conversion efficiency and operational stability are directly relevant for commercial solar cell and sensor applications. These datasets could attract interest from renewable energy and advanced materials companies.
3. Modeling and Simulation Data: Insights into interface engineering and strain effects could inform the design of next-generation hybrid material systems, potentially leading to patents or licensing opportunities.

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

There are no existing 3rd party agreements that restrict the exploitation or dissemination of the data to be used or generated in this project. All datasets, including experimental results, device performance data, and modeling outputs, will be freely available for academic dissemination and in compliance with KU Leuven on open science and data sharing.

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

There are no legal issues, such as intellectual property rights or ownership, that need to be managed for the data used or generated in this project. All datasets, including experimental results, device performance metrics, and modeling outputs, will be owned and managed in accordance with KU Leuven. The data will remain open for academic use and dissemination.

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).

To ensure data remains understandable and usable for both current and future users, the following approach will be implemented for capturing accompanying information:

1. Documentation Standards:
    - Comprehensive metadata will be recorded for all datasets, including experimental procedures, equipment settings, calibration details, and data analysis methods.
    - Metadata will follow standardized formats, ensuring compatibility with institutional and open-access repositories.
2. Electronic Lab Notebooks (ELNs):

    - All experimental procedures, observations, and results will be recorded in a digital format using an Electronic Lab Notebook (ELN) provided by KU Leuven. ELNs ensure traceability, version control, and easy access to data.
3. README Files:
    - Each dataset will include a README.txt file outlining the purpose, structure, and methodology of the data. This file will provide clear instructions for interpreting the data and its metadata.
4. Version Control and Code Documentation:
    - Computational scripts and models will be documented using inline comments and accompanied by a codebook.tsv file that describes the variables, parameters, and expected outputs. Version control tools like Git will be used to track changes and maintain reproducibility.
5. Centralized Storage:
    - All documentation will be stored alongside data in a centralized repository with appropriate folder structures to ensure ease of navigation. Documentation will include detailed descriptions of file naming conventions, units of measurement, and any preprocessing steps.
6. Future Usability:
    - To ensure long-term usability, data and documentation will adhere to FAIR principles (Findable, Accessible, Interoperable, Reusable). This will make datasets understandable and usable by other researchers, even beyond the project team.

By combining robust metadata, detailed procedural documentation, and modern tools like ELNs, the project ensures that data is well-organized, reproducible, and accessible for both immediate use and future research needs.

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.

- Yes

A metadata standard will be used to ensure data is easier to find and reuse. The project will follow the Dublin Core Metadata Standard, which is widely adopted for documenting datasets in research repositories.

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)
- Large Volume Storage
- Personal network drive (I-drive)

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?

To ensure that the data are securely stored and protected from unauthorized access or modification, the following measures will be implemented:

1. Access Control:
    - Data will be stored on Personal network drive (I-drive), OneDrive (KU Leuven), and Large Volume Storage, all of which are protected by KU Leuven's secure authentication system, including multi-factor authentication.
    - Access permissions will be strictly managed, with only authorized project members granted access based on their roles.
2. Encryption:
    - Data stored on OneDrive and Large Volume Storage will be encrypted both during transmission and at rest, ensuring high levels of confidentiality and security.
3. Regular Backups:
    - The Personal network drive (I-drive) and Large Volume Storage are automatically backed up daily by KU Leuven IT services, providing protection against accidental data loss or corruption.
    - Additional manual backups will be periodically saved to OneDrive to ensure redundancy.
4. Version Control and Audit Trails:
    - For critical data, version control mechanisms will be used to track changes. This ensures the integrity of the data and allows for the identification and reversal of unauthorized modifications.
5. Institutional Policies and Compliance:
    - All data management practices will comply with KU Leuven's policies on data protection and adhere to GDPR regulations where applicable.

By combining secure storage systems, encryption, and controlled access, the data will remain protected from unauthorized access or modification throughout the project.

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

The expected costs for data storage and backup during the research project are minimal, as the majority of storage solutions are provided by KU Leuven:

1. Data Storage Costs:
    - Personal network drive (I-drive) and OneDrive (KU Leuven): Provided free of charge by KU Leuven for academic use.
    - Large Volume Storage: While the exact cost depends on the volume of data, typical charges are approximately €100–€200 per terabyte per year.
2. Backup Costs:
    - Regular automated backups for I-drive and Large Volume Storage are included as part of KU Leuven IT services and incur no additional charges.
    - Manual backups on OneDrive also incur no cost.
3. Coverage of Costs:
    - Any additional costs for Large Volume Storage will be covered by the bench fee allocated to the project, ensuring seamless data management without compromising the research budget.

The use of KU Leuven-provided resources ensures cost-effectiveness and compliance with institutional data management policies.

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)?

- Shared network drive (J-drive)

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

The expected costs for data preservation during the retention period are minimal due to the use of KU Leuven's institutional storage infrastructure:

1. Costs for Data Preservation:
    - Personal Network Drive (I-drive): No additional cost, as it is provided free of charge by KU Leuven for academic use, including the retention period.
    - OneDrive (KU Leuven): Free for long-term storage of small to medium-sized datasets.
    - Large Volume Storage: Estimated at €100–€200 per terabyte per year, depending on the volume of data. For a retention period of 10 years, the total cost will depend on the final data size.
2. Coverage of Costs:
    - Costs for any additional storage requirements (e.g., Large Volume Storage) will be covered by the project's bench fee or institutional research funds. KU Leuven policies ensure affordable and scalable options for long-term data preservation.

By utilizing KU Leuven's resources, the project ensures compliance with retention policies while minimizing financial impact.

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 embargoed data (temporary restriction)

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

Access to the data will initially be restricted to the project team and authorized collaborators during the research phase. After the relevant research findings are published, the data will be made publicly available through open-access repositories in compliance with KU Leuven's open science policies.
If some datasets need to remain restricted (e.g., raw experimental data with proprietary implications), access will be granted upon request and subject to a data sharing agreement ensuring proper citation and acknowledgment.

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?

- Upon publication of research results

Which data usage licenses are you going to provide?

If none, please explain why.

- CC-BY 4.0 (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.

- 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?

No costs are expected. If any costs occur, they will be covered by the requesting party.

Responsibilities

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

Yujie Gao will be responsible for data documentation and metadata during the project, under supervision of prof. Maarten Roeffaers (supervisor).

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

Yujie Gao will be responsible for data storage and back-up during the project, under supervision of prof. Maarten Roeffaers (supervisor).

Who will manage data preservation and sharing?

Prof. Maarten Roeffaers (supervisor) will be responsible for data preservation after the end of the project. Yujie Gao will be responsible for data sharing during the project, under supervision of Prof. Maarten Roeffaers. Prof. Maarten Roeffaers will be responsible for data sharing after the end of the
project.

Who will update and implement this DMP?

Yujie Gao will update and implement this data management plan througout the project, under supervision of Prof. Maarten Roeffaers (supervisor).