DMP title

Project Name Functional Engineering of Metal Halide Perovskites: A Nonlinear Optical Study (FWO DMP) - DMP title

Grant Title 1S92622N

Principal Investigator / Researcher Giorgia Rizzi

Description Crystalline materials are essential components of modern technology, so it is necessary to know how to control their preparation in order to design increasingly efficient devices. Structural polymorphism is the ability of a material to adopt multiple lattice structures with different functional properties (chemical, electrical, and optical). This PhD project focuses on metal halide perovskites(MHPs) and how to gain control over their structure by calibrating the experimental parameters such as synthesis method, composition, morphology and temperature. In fact, MHPs exhibit interesting electro-optic properties that strictly depend on their crystalline structure. In particular, we focus on studying ferroelectricity (FE) and on the characterization of the crystal phase. The primary technique used to study of FE is second harmonic generation microscopy, which allows both to determine FE presence and to perform structural imaging of MHPs. By combining this technique with other nonlinear optical probes, such as third harmonic generation and multiphoton microscopy together with harmonic light scattering, it's possible to obtain the most complete structural characterization achievable by optical means. The use of other techniques, such as XRD, SEM, absorption and emission spectroscopy will help establish how the electro-optic properties relate to crystal structure, so it will be possible to determine how to better exploit MHPs in solar cells, LEDs or chemical sensors.

Institution KU Leuven

1. General Information

Name applicant

Giorgia Rizzi

FWO Project Number & Title

1S92622N - Functional Engineering of Metal Halide Perovskites: A Nonlinear Optical Study

Affiliation

- KU Leuven

Science, Engineering and Technology Group, Chemistry, Kulak Kortrijk Campus

2. Data description

Will you generate/collect new data and/or make use of existing data?

- Generate new data
- Reuse existing data

Describe in detail the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a table (see example) or as a data flow and per WP or objective of the project. If you reuse existing data, specify the source of these data. Distinguish data types (the kind of content) from data formats (the technical format).

The research will generate data as material samples via synthesis and preparation. These materials will be in the form of solutions or crystals and powders, both in dry form and in nonsolvent suspension. The samples will be stored in sealed glass or plastic recipients.

The synthesis and preparation procedures and the researcher's experimental observations will be noted in laboratory notebooks, generating analog data. Analog lab data will be copied in an electronic lab-book with appropriate reference to the material samples.

For comparison reasons and referencing, existing data may be used. This data can be both as materials previously synthesized/prepared or as information (eg. absorption and emission spectra, PXRD patterns, etc.) shared in scientific publications or specific databases (eg. The Cambridge Structural Database).

Experimental data will be collected for material characterization, in a variety of file formats (see bellow).

Multiple data files will be generated, organized in a well-defined structured folder with analysis results and detailed statistical analyses. All the digital files will cointain the specific abbreviation

of the analyzed sample in the name (eg. GRXX, where GR are the initials of the researcher that prepared the sample and XX is the number of the page of the laboratory notebook in which the sample's preparation procedure is written).

Below, the list the file types for the raw data, processed/analyzed data and final data (published).

Setup that generates the data	**File type - Raw data**	**Contains metadata?**	**File type - Analysis**	**Contains metadata?**	**File type publication**
SHG microscopy	AIST, TXT, LSF	yes	TIFF, BMP, JPG	yes	TIFF, PPT, PDF,BMP
Wide-field SHG microscopy	ASC, SIF	yes	MAT, ORG	yes	PDF, PPT, TIFF, JPG, PSD, PNG
SEM microscopy	TIF, TXT	yes	BMP, XLSX	yes	PDF, JPG, PNG
EDS	BMP, EMF, TXT	yes	PDF	no	PDF, JPG
XRD diffraction	TXT, Rigaku RAW, DAT, Diffrac Plus Raw	yes	TXT, DAT	yes	TXT, PPT, PDF
optical absorption and emission spectroscopy	ASC, SP, FS, TXT, XLSX, SP, RSC, OPJ	yes	TXT, SP, OPJ, XLSX	yes	PDF, PPT, TIFF, JPG, PSD, PNG, DOCX
piezo-response force microscopy	STP, MP, IBW, TXT	yes	TIFF, BMP, JPG	yes	TIFF, PPT, BMP, PDF
Hyper-Rayleigh scattering	TXT	yes	OPJ, TXT	yes (metadata via additional file)	JPG, TIFF, BMP, PNG, DOCX

We estimate a total data size of **500Gb** for the entire project.

3. Legal and ethical issues

Will you use personal data? If so, shortly describe the kind of personal data you will use. Add the reference to your file in KU Leuven's Register of Data Processing for Research and Public Service Purposes (PRET application). Be aware that registering the fact that you process personal data is a legal obligation.

- No

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, add the reference to the formal approval by the relevant ethical review committee(s)

- No

Does your work possibly result in research data with potential for tech transfer and valorisation? Will IP restrictions be claimed for the data you created? If so, for what data and which restrictions will be asserted?

- Yes

The generated data restriction is in accordance with the framework policy of the university. When potential data and results that can lead to tech transfer and valorisation are collected, LRD will be consulted for support and advice.

Do existing 3rd party agreements restrict dissemination or exploitation of the data you (re)use? If so, to what data do they relate and what restrictions are in place?

- No

4. Documentation and metadata

What documentation will be provided to enable reuse of the data collected/generated in this project?

In order to make sure all the data collected and stored will be reliable and reproducible, a text document describing the exact expeimental conditions, including date, time, location of measurements, instruments, sample preparation protocol and measurement parameters etc. This file will be kept in the same folder where the data is stored.

In addition, data will be stored in a folder per experimental setup, the type of investigated system and the corresponding date.

The names of the files will be structured in a comprehensible way. The name of each file will contain the specific abbreviation of the analyzed sample in the name (eg. GRXX, see section 2). In this way, by tracking the corresponding logbook/lab-book notes, each file can be easily found on the local computers controlling the setup and on the server of the laboratory.

For the materials, a list of samples and the location where these are stored will be kept in researcher's logbook. A description of the sample's characteristics (e.g. sample name, solvent, quantity, date, concentration) will be added to allow rapid identification and reuse.

Will a metadata standard be used? If so, describe in detail which standard will be used. If no, state in detail which metadata will be created to make the data easy/easier to find and reuse.

- No

There is no formal metadata standard. However, the standardized steps described in section 4.1 will ensure that the data is easy to find and reuse.

5. Data storage and backup during the FWO project

Where will the data be stored?

Data will be firstly collected and kept at the local desktops of the instruments. For analysis purposes some data will also be copied on the researcher's computer and personal storages such as portable hard disks. In any case, a backup copy of the raw data will be automatically made on the servers of ICTS - Standard. The data will be also backed-up in a secure server space in KULAK. All the data will also be organized and saved in the researcher's personal cloud backup storage (2TB) provided by KU Leuven.

For the materials, the recipients containing samples will be sealed, labelled and stored in a cabinet for chemicals. Samples containing materials sensitive to environment (perovskites) will be stored in inert atmosphere or under dry nonsolvent to avoid degradation. Since perovskites are also sensitive to light, they will be stored in dark recipients to avoid contact with light.

Laboratory notebooks will be stored in the office C754 at the Kulak campus. The content of the lab-notebook will be copied in electronic lab-books with appropriate reference to the obtained data. The electronic lab-book will be stored in a cloud service according to the GDPR of EU. The data will be backed-up in a secure server space in KULAK

How is backup of the data provided?

The data will be mirror stored on the university's central servers (large volume storage at ICTS)

with automatic daily back-up procedures.
The produced materials will be stored for at least one year. After that time, only the samples that do not undergo degradation (not useful anymore) or of particular relevance will be stored.

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

The amount of data that will be generated in this project should not exceed a few hundreds GBs, which is small enough to be stored in local computers and on the data server of the laboratory.
The amount of space in the cabinet used as a storage for samples is currently sufficient.

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

The costs for digital data storage and back up are covered by the (co-)promotors.
The costs for eventual extra chemical storage cabinets will be covered by the project's supervisor.

Data security: how will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

The identifiable data files from this project will be managed, processed, and stored in a secure environment. The data transfer with the ICTS - Standard Storage Solutions provided by KU Leuven is done over an encrypted connection. The data is encrypted with a 256-bit SSL.
The place where the materials are stored is only open to the IRF members via badge access.

6. Data preservation after the FWO project

Which data will be retained for the expected 5 year period after the end of the project? In case only a selection of the data can/will be preserved, clearly state the reasons for this (legal or contractual restrictions, physical preservation issues, ...).

All data will be stored in ICTS - Standard Storage Solutions provided by KU Leuven (with automatic backup procedures) for at least 10 years, conform the KU Leuven RDM policy unless there will be legal or contractual restrictions in the case of tech transfer or valorisation events. Close consultation with LRD and ICTS will be conducted in those cases to ensure IP and data security.
For materials, only the samples that preserve their original physical and chemical properties will be retained after the end of the project. Samples that have unstable properties, meant to be use for a limited number of experiments or for limited lifetime will not be preserved or preserved for at least 1 year after the preparation depending on the case.

Where will the data be archived (= stored for the longer term)?

The data will be archived on the university's large volume storage servers (with automatic backup procedures) for at least 10 years, conform the KU Leuven RDM policy.
The materials will be stored in special designed laboratory cabinets, in the case of stable samples.

What are the expected costs for data preservation during the retention period of 5 years? How will the costs be covered?

The costs will be covered by the project's (co-)promotors.

7. Data sharing and reuse

Are there any factors restricting or preventing the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

- Yes. Specify:

KU Leuven holds the IPR.

Which data will be made available after the end of the project?

All the data associated to published articles, conference abstracts and posters will be made available after publication or the end of the project, as requested by the FWO open access

obligation.
The data can also be made available via restricted access upon request of an individual (e.g. a researcher who intends to reproduce an experiment) after agreement of the project promotors.

Where/how will the data be made available for reuse?

- In an Open Access repository
- In a restricted access repository
- Upon request by mail

Published data:

- will be made available in an Open Access repository (Lirias, KU Leuven)
- Raw data, dataset and processed data can be made available upon request by email.

Unpublished data:

- will be available upon request and after approval of the (co-)promotors.

Data with IP potential:

- will undergo an embargo period until IP is secured
- or will be available in a restricted access repository

When will the data be made available?

The results will be disseminated in journals with policy requiring disclosure upon.
Data associated to publications will be made available upon publication. Results with IP potentials will go through an embargo period until IP is secured.

Who will be able to access the data and under what conditions?
Published data will be open to the scientific community.
The unpublished data can be accessible upon request and with the prior authorization of the (co-)promotors.

What are the expected costs for data sharing? How will the costs be covered?
There will be no costs associated with data sharing.

8. Responsibilities
Who will be responsible for data documentation & metadata?
The PhD researcher and the supervisor of the project (Stijn Van Cleuvenbergen)

Who will be responsible for data storage & back up during the project?
The supervisor of the project.

Who will be responsible for ensuring data preservation and reuse ?
The supervisor of the project.

Who bears the end responsibility for updating & implementing this DMP?
The PhD researcher and the supervisor of the project.