DMP title

Project Name IDN: Understanding and boosting the performance of organic thermoelectrics by a tailored molecular design guided by experiments and simulations - DMP title

Project Identifier IDN OTE

Grant Title IDN/21/012

Principal Investigator / Researcher Francisco Molina Lopez

Description The purpose of the data generation (mostly lab experimental data) is the study of the properties and performance of the materials and devices to be developed in the project, as well as the generation of the necessary protocols and set-ups needed for such study. Collecting and interpreting these data will lead directly to the objective of the project of developing flexible organic thermoelectric devices with improved performance.

Institution KU Leuven

1. General Information

Name of the project lead (PI)

Francisco Molina-Lopez

Internal Funds Project number & title

IDN/21/012: Understanding and boosting the performance of organic thermoelectrics by a tailored molecular design guided by experiments and simulations.

2. Data description

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

- Generate new data

2.2. What data will you collect, generate or reuse? Describe the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a numbered list or table and per objective of the project.

Type of data	Format	Volume	How created	WP
Materials datasheet	.pdf	1-10 MB	To be received from suppliers.	1-4
Standard Operating Procedures	.docx, .mp4, .AVI	10 GB	Written or filmed by the researcher.	1-4
Microscopy (optical and SEM) images	.tif	1 GB	Digital microscope Keyence and SEM microscope images printed films. Optical microscope with polarizers.	1-4
TEM microscopy	.tif	100 MB	TEM microscope at Nanocenter	1-4
Energy-dispersive X-ray spectroscopy (EDS) peaks and mapping images	.docx	1-10 MB	Images of printed films.	1-4
Lab XRD peak images	.tif, .raw, .njc	1-10 MB	XRD peak images of printed films. The raw data can be handled with the equipment software and exported as an image.	1-4

Synchrotron XRD (GI)WAXD	.tif, .xls, .raw	100 MB	Data generated in the DUBBLE beamline BM26, at the ESRF facilites in Grenoble, France. A custom-built software will be used to analyze the measured data.	1-4
Synchrotron XRD (GI)SAXD	.tif, .xls, .raw	100 MB	Data generated in the DUBBLE beamline BM26, at the ESRF facilites in Grenoble, France. A custom-built software will be used to analyze the measured data.	1-4
Phase change and crystallinty	.tif, .xls	1-10 MB	DSC	1-4
UV-Vis(-IR) spectroscopy (polarized)	.tif, .xls, .raw	1-10 MB	Measured at the Dept. of Chemistry with specialized equipment.	1-4
Raman spectroscopy	.tif, .xls, .raw	1-10 MB	Measured at Nanocenter with specialized equipment.	1-4
AFM	.tif, .xls	1-10 MB	Measured at Dept. of Chemitry. Specialized software included in the AFM will be used to analyze the data.	1-4
XPS/UPS	.tif, .xls	1-10 MB	Measured in collaboration with Prof. R. Ameloot	2-4
Electrical conductivity at different temperatures	.xls	1-10 MB	File to be produced by the dedicated setup LSR-3 (Linseis).	1-4
Seebeck coefficient at different temperatures	.xls	1-10 MB	File to be produced by the dedicated setup LSR-3 (Linseis).	1-4
Thermal conductivity at different temperatures	.xls	1-10 MB	File to be produced by a light flash analyzer and DSC.	1-4
Electrical and Seebeck conductivity upon bending at room temperature (optional)	.xls	1-10 MB	File to be produced by a dedicated setup using Matlab or LabView to interface the measuring equipment. Or if possible with a dynamic mechanical analyzer (DMA).	4

Layouts of inkjet printed materials (optional)	CAD files & .bmp	100 MB	Designed by the researchers in any photo editor or in the software of the Dimatix printer.	1-4
Videos with demos	.mp4 & .AVI	10GB	Videos showing working demos and bending tests.	1-4
Relevant reviewed literature	.pdf, .bib	1-10 MB	Articles will be available at the KU Leuven digital library. The articles may be stored in pdf and the selection of articles can be exported as a .bib file using the reference manager Mendeley.	1-4
Lab books with written details about the different process trials, results, and observations.	Written in paper	1drawer	Written by the researchers in the lab. To be kept for 5 years.	1-4
Physical samples	Physical	50 L	Fabricated by the researchers in the lab. To be kept for 5 years.	1-4
Inputs and outs of computer Simulations	Specialized formats	10GB	Data to be produced by Prof. D. Escudero from Dept. of Chemistry	1-4
Computer codes and scripts	Specialized formats	1GB	Data to be produced by Prof. D. Escudero from Dept. of Chemistry	1-4

3. Ethical and legal issues

3.1. Will you use personal data? If so, shortly describe the kind of personal data you will use. Add the reference to the file in KU Leuven's Record of Processing Activities. Be aware that registering the fact that you process personal data is a legal obligation.

No

3.2. 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

3.3. Does your research 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

If the data has potential for valorization, the concept/material/device will be registered first and published afterward. The data will be reused under the licence Creative Commons Attribution-NonCommercial-NoDerivs (CC-BY-NC-ND).

3.4. 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 regarding

reuse and sharing are in place?

No

4. Documentation and metadata

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

Our group joined the pilot program, iRODS, developed by the Research Data Management Competence Center (RDM-CC) at KU Leuven to standardize data and metadata. This allows us to define metadata for different data collections. For instance, we can assign fields like "user", "project", "instrument", "date" to each of our files. The files will be stored in a university-owned server, free of charge and without space limitation. "ReadMe" txt files will be provided as legends for the metadata fields and attributes.

Regarding other kinds of generated data:
1. Lab books will be classified by author and project. The inputs written in the lab books will be organized by date.
2. Microscopy images will be accompanied by a scale bar and a txt "ReadMe" file detailing the conditions of the measurement (light intensity, contrast, magnification, etc.). The conditions will be also annotated in the lab books.
3. Standard equipment such as XRD, SEM, and EDS generates a metadata file with the measuring conditions. This file will be retained. The conditions will be also annotated in the lab book.

For the research data concerning the simulation work (D. Escudero):

During research, data will be stored on computers belonging to the Quantum Chemistry and Physical Chemistry Division (QCPC) and to the Flemish Supercomputing Centre. Key data will always be backed up regularly to avoid loss of data (i.e., this is done on a daily basis in our cluster at the QCPC). Generally to unambiguously trace and organize data; the data arising from the simulations (inputs&outputs) will be collected in separate folders per simulation test, including a txt file with a clear description of what the data represent and how they were generated. A common protocol to name and store data for this project will be set up among all project members. Scripts, codes, input&output files will unambiguosly display date of creation and who generated the data.

4.2. Will a metadata standard be used? If so, describe in detail which standard will be used. If not, state in detail which metadata will be created to make the data easy/easier to find and reuse.

No

The data will be stored in folders named as the user. Then, each user will create its own folder structure. Metadata referring to the date, project, equipment, type of data (paper, raw data, presentation, etc.) ... will be assigned to each file. This feature is enabled by the iRODS platform put in place by KU Leuven.

The metadata attributes used for search are summarized in txt "ReadMe" files.

We will name the successive file versions as xxx_V1, xxx_V2, etc. Also, the date when the file was generated will be used to track the version.

The relevant datasets (except for some unpublished SOPs and other files related to the group know-how) will be uploaded in OpenAIRE or Zenodo under a license. Hence, they will receive a DOI for identification.

Concerning the simulation work (D. Escudero): The PI has considerable expertise in curating computational chemistry research data with these types of approach. All data (appropriately collected and classified with a clear description of what the data represent and how they were generated) will be preserved for at least 10 years (this is the standard protocol at the QCPC division.

5. Data storage and backup during the project

5.1. Where will the data be stored?

All the data generated by Pof. Molina-Lopez's group will be first produced and stored in personal computers in the Department of Materials Engineering (MTM) drives, and immediately shared in iRODS.

The KU Leuven Box space will be used to share data with external visitors and master students. Each researcher will be responsible to transfer the data from their personal computer to the shared spaces.

The others PIs will follow their usual proceducer to store data. For instance, for the simulation work (D. Escudero): Full output from all calculations is very voluminous, but the field has standard protocols for collecting the key data. Specifically, data will be stored in our computers belonging to the Quantum Chemistry and Physical Chemistry Division (QCPC, KU Leuven) and on the data storage services of the Flemish Supercomputing Centre (VSC).

5.2. How will the data be backed up?

The iRODS and BOX systems provides continuous and automatic backups.

For the simulation work (D. Escudero): Automatic daily back-up procedures are ensured at both our QCPC cluster as well as at the VSC facilities.

5.3. 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, virtually unlimited.

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

There are no extra costs expectedf for MTM.

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

Each university-associated computer requires a password for logging in. This password must be changed every year. Access to the iRODS and KU Leuven Box space is also protected by a password. No sensitive data will be handled in this project. Each research will have access to their own data and the PI (Francisco Molina-Lopez) will have access to the data of every member of the project.

The other PIs will manage their data following their usual procedures.

6. Data preservation after the end of the project

6.1. Which data will be retained for the expected 10 year period after the end of the project? If only a selection of the data can/will be preserved, clearly state why this is the case (legal or contractual restrictions, physical preservation issues, ...).

Physical data in the form of lab books and samples will be retained for 5 years. Most samples will degrade with time and will not be usable after 5 years in any case. Due to space restrictions, lab books will be retained also for 5 years. Digital data will be retained for 10 years.

6.2. Where will these data be archived (= stored for the long term)?

Samples and lab books will be stored for 5 years in dedicated cabinets and drawers in the labs. Digital data will be retained for 10 years on internal KU Leuven data storage facilities. Storing in a repository (such as Zenodo) will be considered.

6.3. What are the expected costs for data preservation during these 10 years? How will the costs be covered?

NA

7. Data sharing and re-use

7.1. 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 or because of IP potential)?

Unpublished data related to specific SOPs, and non-essential for reproducibility of claimed results will not be shared.

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

The full dataset (except for some unpublished SOPs and other know-how-related files) will be uploaded in Zenodo under a CC-BY license.

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

- In an Open Access repository
- Upon request by mail

7.4. When will the data be made available?

- Upon publication of the research results
- After an embargo period. Specify the length of the embargo and why this is necessary

Published but embargoed data can be shared upon personal request by email. These data will be deposited in the Lirias KU Leuven repository. The embargo period is usually 6 months for most journals in the field.

7.5. Who will be able to access the data and under what conditions?

The data will be available to anyone for any purpose, provided that they give appropriate credit to the creators. However unpublished SOPs and other know-how-related knowledge, which is non-essential for the reproducibility of claimed results will not be shared.

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

NA

8. Responsibilities

8.1. Who will be responsible for the data documentation & metadata?

Francisco Molina-Lopez, the PI of the project, will be responsible for data documentation produced at MTM.

Daniel Escudero and Guy Koeckelberghs, the co-promotors in the project, will be responsible for data documentation produced at the department of Chemistry.

8.2. Who will be responsible for data storage & back up during the project?

Each researcher will be responsible to transfer the data to the iRODS shared folders and/or Box shared folders. The backup of the data is automatic in those platforms.

8.3. Who will be responsible for ensuring data preservation and sharing?

Francisco Molina-Lopez, the PI of the project, will be responsible for data preservation and reuse at MTM.

Daniel Escudero and Guy Koeckelberghs, the co-promotors in the project, will be responsible for data preservation and reuse at the department of Chemistry.

8.4. Who bears the end responsibility for updating & implementing this DMP?

The end responsibility for updating and implementing the DMP is with the supervisors (promotor and co-promotors).