

DMP title

Project Name EOS CONNECT KUL - DMP title

Project Identifier G0J4922N

Grant Title G0J4922N

Principal Investigator / Researcher Lino da Costa Pereira

Project Data Contact +32 16 32 01 76, lino.pereira@kuleuven.be

Description This project, titled "Caloritronics in Magnetic Weyl Semimetals" (CONNECT), is funded under the EOS program of the FWO - Research Foundation Flanders. The project has partners from the KU Leuven, UC Louvain, IMEC. The DMP covers the management of the data produced by the two KUL partners, namely the Quantum Solid State Physics (QSP) division (PI: Lino da Costa Pereira; co-PI: Margriet Van Bael) and the Surface and Interface Engineered Materials (SIEM) division (co-PI: Francisco Molina-Lopez). The CONNECT project consists of the synthesis of high-quality magnetic Weyl semimetals as well as theoretical modeling and experimental studies of their coupled properties, aiming to reach a thorough understanding of spin, heat and charge currents in these materials. The specific roles of the KU Leuven partners consist of: (i) synthesis of some of the Weyl semimetal materials foreseen under CONNECT; (ii) experimental studies of the structural, elemental, electronic, topological and magnetic properties of all the Weyl semimetal materials foreseen under CONNECT, (iii) solvent-less patterning of electrodes to define a measurable device.

Institution KU Leuven

1. General Information

Name applicant

PI: Lino da Costa Pereira (QSP division)

co-PI: Margriet Van Bael (QSP division)

co-PI: Francisco Molina Lopez (SIEM division)

FWO Project Number & Title

G0J4922N - "Caloritronics in Magnetic Weyl Semimetals" (CONNECT)

Affiliation

- KU Leuven

The project has partners from the KU Leuven, UC Louvain, IMEC, This DMP covers the management of the data produced by the two KU Leuven partners, namely the Quantum Solid State Physics (QSP) division and the Surface and Interface Engineered Materials (SIEM) division.

2. Data description

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

- Generate new 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).

| Type of data | Format | Volume | How created | WP |
|----------------------------------|-------------------|---------|--------------------------------------------------------------------------------------------------------|------|
| Materials datasheet | .pdf | 1-10 MB | To be received from suppliers. | 4 |
| Standard Operating Procedures | .docx, .mp4, .AVI | 10 GB | Written or filmed by the researcher. | 1, 4 |
| Microscopy (optical, SEM) images | .tif | 1 GB | Digital microscope Keyence and SEM/TEM microscope images of films. Optical microscope with polarizers. | 1, 4 |

| | | | | |
|---------------------------------------------------------------------|------------------|----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| TEM microscopy | .tif | 100 MB | TEM microscope at Nanocenter | 1 |
| Energy-dispersive X-ray spectroscopy (EDS) peaks and mapping images | .docx | 1-10 MB | Images of films. | 1, 4 |
| Lab XRD peak images | .tif, .raw, .njc | 1-10 MB | XRD peak images of films. The raw data can be handled with the equipment software and exported as an image. | 1 |
| SQUID measurements | ASCII | 1-100 MB | Magnetometry measurements performed using a SQUID magnetometer. | 2 |
| XMCD and ARPES measurements | ASCII | 1-2 GB | Measurements performed in international synchrotron radiation facilities. The data is kept and managed on the facility itself following local RDM policies, but is also copied onto KU Leuven local servers, in order to ensure that the present DMP of this project is followed. | 2, 3 |
| STM and STS measurements | ASCII | | Scanning tunneling microscopy and spectroscopy using the various available setups. | 1, 2 |
| AES, XPS, XRD measurements | ASCII | | Standard material characterization performed in the various available setups. | 1 |
| Phase change and crystallinity | .tif, .xls | 1-10 MB | DSC | 1 |
| AFM | .tif, .xls | 1-10 MB | Specialized software included in the AFM will be used to analyze the data. | 1 |
| Electrical conductivity at different temperatures | .xls | 1-10 MB | For both semimetal films and electric contacts. File to be produced by the dedicated setup LSR-3 (Linseis). | 4 |

| | | | | |
|-----------------------------------------------------------------------------------------------|------------------|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| Seebeck coefficient at different temperatures | .xls | 1-10 MB | For the semimetal films. File to be produced by the dedicated setup LSR-3 (Linseis). | 4 |
| Thermal conductivity at different temperatures | .xls | 1-10 MB | File to be produced by a light flash analyzer and DSC. | 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 | 1 drawer | 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 |

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

Although tech transfer and valorisation are not direct goals of this project, if such an opportunity presents itself, it will be discussed among the PIs involved in the project. The conclusions of that discussion will be appended to this data management plan. As a general principle, the concept/material/device will be registered first and published afterwards; the data will be reused under the licence Creative Commons Attribution-NonCommercial-NoDerivs (CC-BY-NC-ND).

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?

Regarding data collected by researchers from the QSP division:

During each experiment, a detailed logbook will be used (different logbooks for the different experimental setups). These logbooks will contain the date, a brief description of the performed experiment, the parameters used for each measurement, as well as the names of all the saved files.

The names of the files will be structured in a comprehensible way:
system studied/date/main parameters used

In addition, data will be stored in a folder per experimental setup, the type of investigated system and the corresponding date. In this way, by tracking the corresponding logbook notes, each file can be easily found on the local computers controlling the setup and on the server of the laboratory.

The analysis files will contain notes describing the analysis procedure and mention which original data files are included. A readme file describing the goal of the experiment and the analysis procedure will be stored in the folder where the data is saved.

Regarding data collected by researchers from the SIEM division:

The research 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.

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

Regarding data collected by researchers from the QSP division:

Regarding the experimental data, in the relevant research field, there is no formal metadata standard. However, the standardized steps described in this section 4 will ensure that the data is easy to find and reuse.

Regarding data collected by researchers from the SIEM division:

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.

5. Data storage and backup during the FWO project

Where will the data be stored?

Regarding data collected by researchers from the QSP division:

The data, including raw data, analysis files, as well as reports and electronic logbooks, will be saved on local computers. The data stored on these computers is backed-up daily on a local server. A duplicate of this back-up is made on the back-up server. All researchers involved in the

project will have access to the corresponding folder.

Regarding data collected by researchers from the SIEM division:

All the data 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.

How is backup of the data provided?

Regarding data collected by researchers from the QSP division:

The data stored on the local computers is continuously and automatically backed-up on local servers.

Regarding data collected by researchers from the SIEM division:

The iRODS and BOX systems provides continuous and automatic backups.

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 hundred GBs, which is small enough to be stored in local computers and on local servers.

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

The costs are minimal and are covered by the project budget.

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

Regarding data collected by researchers from the QSP division:

The data will be systematically transferred to the local server, with restricted access (managed by the IT responsible). Only the (co-)promotors and involved researchers have access to the shared folders where the data, analysis files and reports will be stored. Also, credentials are required to log in to local computers in the laboratories.

Regarding data collected by researchers from the SIEM division:

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 researcher will have access to their own data and the PI of the SIEM division (Francisco Molina-Lopez) will have access to the all the project data generated by researchers of the SIEM division.

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, ...).

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. Due to space restrictions, lab books will be retained also for 5 years. Digital data will be retained for 10 years.

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

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

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

The system and cost allocation described in section 5.4 will also be used for data preservation after the project ends. Costs are expected to be negligible and will be covered by other running

projects from the involved groups (in case of no running projects, accumulated reserves will be used).

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)?

- No

There are no legal restrictions or restriction related to IP potential.

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

All data can be made available, for example if requested by the editor or publisher of a scientific journal or upon request of an individual (e.g. a researcher who intends to reproduce an experiment).

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

- In an Open Access repository
- In a restricted access repository

Upon request and after the agreement of the project's PIs, all data can be made available on an open repository (e.g. Zenodo), for example if requested by the editor or publisher of a scientific journal or via restricted access upon request of an individual (e.g. a researcher who intends to reproduce an experiment).

When will the data be made available?

- Upon publication of the research results

After the research results have been published and after agreement of the PIs (with a possible embargo time no longer than one year after the publication of the research)

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

All involved researchers will have access to all the data. Upon request and after agreement of the PIs, access to the data can be granted to other individuals/parties.

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

There will be no costs for data sharing. Since the volume of most files is not too large, freeware can be used to transfer and share the files.

8. Responsibilities

Who will be responsible for data documentation & metadata?

The PIs of the project: Lino da Costa Pereira (QSP), Margriet Van Bael (QSP), Francisco Molina Lopez (SIEM).

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

The PIs of the project, together with the IT responsables of the research groups, who are responsible for the implementation of the storage and operation of the local servers.

Who will be responsible for ensuring data preservation and reuse ?

The project PIs.

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

The PIs of the project bear the end responsibility of updating & implementing this DMP: Lino da Costa Pereira (QSP), Margriet Van Bael (QSP), Francisco Molina Lopez (SIEM).